Hydrodynamic and Water Quality Simulation of Fecal Coliforms in the Lower Appomattox River, Virginia

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

Master of Science

in

Civil Engineering

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September 9, 2004
Blacksburg, VA

Keywords: hydrodynamic modeling, water quality modeling, tidal estuary.

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Abstract

The Virginia Department of Environmental Quality (VADEQ) under the direction of the United States Environmental Protection Agency (USEPA) has listed the lower Appomattox River as impaired because it violates current water quality standards for fecal coliforms. To advance the analytical process, by which various scenarios for improving water quality within the estuary are examined, an array of computer-based hydrodynamic and water quality models were investigated. The Dynamic Estuary Model (DYNHYD5), developed by USEPA, was used to simulate hydrodynamics within the lower Appomattox River. The Water Quality Analysis Simulation Program (WASP6.1), also developed by USEPA, was employed to perform water quality simulations of fecal coliforms. Also, a detailed literature review examined DYNHYD5 and WASP6.1 model theory, computer-based model solution techniques, and background hydrodynamic theory.

DYNHYD5 sensitivity analysis showed that the model was most responsive to tidal heights (seaward boundary conditions) both upstream and downstream within the model network. Specific model parameters were varied during calibration until modeled water surface elevations converged on observed water surface elevations. A goodness-of-fit (r^2) value of 0.749 was determined with linear regression analysis for model calibration. DYNHYD5 input parameter validation was performed with additional observations and a goodness-of-fit value of 0.829 was calculated.

Through sensitivity analysis, WASP6.1 proved to be most responsive to coliform loading rates in the downstream direction and boundary concentrations in the upstream direction. With these results, WASP6.1 input parameters were calibrated against observed fecal coliform concentrations. A goodness-of-fit (r^2) value of 0.573 was determined with linear regression analysis for model calibration. WASP6.1 input parameter validation was performed with additional observations and a goodness-of-fit value of 0.0002 was calculated.

Model results suggest that hydrodynamic model calibration and validation can be improved with additional tidal height observations at the downstream seaward boundary. Similarly, water quality model calibration and validation can possibly be improved with the aid of detailed, time-variable coliform concentrations at the downstream seaward boundary. Therefore, it is recommended that a water quality sampling station and tidal stage recorder be installed at the confluence of the Appomattox and James Rivers to provide for further testing of estuary hydrodynamic and water quality models.

Acknowledgements

As my time at Virginia Tech comes to a close, there are numerous people I would like to thank for their continued encouragement and support over the past 2 years. My journey can be likened to that of a roller coaster ride. It has consisted of numerous ups and downs as well as a few twists, turns, and loops. My time-spent working feels like it has come and gone with a few blinks of the eye, and I'm reminded of the old saying: "time flies while you're having fun." With that said, I'm back to the business at hand.

First and foremost, I would like to thank Dr. David Kibler and Dr. G. V. Loganathan for encouraging me to pursue graduate school. In addition, a special acknowledgement to Dr. Kibler for getting me on board (so to speak) with this research as well as for your encouragement, support, and guidance throughout the entire process. Also, I would like to express my gratitude to my thesis committee: Dr. Daniel Gallagher, Dr. David Kibler, and Dr. G. V. Loganathan.

I would like to thank the entire staff at MapTech, Inc. (Blacksburg, VA) for providing me with a desk to work and for treating me as one of their own. A special thanks to Mr. Phil McClellan for providing me with this research opportunity. Rob Burgholzer, thanks for bringing me up to speed on HSPF as well as for all the data and support during the tiresome hours spent modeling. Matthew McClellan, thanks for navigating the boat during bathymetry data collection. Emily Smith, thanks for demystifying the ArcView software. Dr. Jim Kern, thanks for the support during model calibration and validation. Dr. Vernon Shanholtz, thanks for bringing me up to speed on FORTRAN. Dr. Youtong Fu, thanks for all of the modeling advice and suggestions. To the rest of the MapTech staff, thanks for everything.

I would like to thank Mr. Tim Wool (USEPA) for answering my numerous questions concerning WASP6.1 and for recompiling DYNHYD5 to be used this research. In addition, I would like to express my gratitude to Dr. Robert Ambrose (USEPA) for his support as well as insight into the DYNHYD5 software.

To my friends in Hydrosystems at Virginia Tech, thanks for making the workdays enjoyable. Troy Biggs, Kevin Young, Jon Ladd, and Joshua Joseph, thanks for all the encouragement, support, and laughs. Special thanks to Troy Biggs for uncomplicating the ArcGIS software as well as for providing a set of ears for griping and complaining.

I would like to thank my family: Mom, Dad, and Bo for their continued support and encouragement that remained steadfast my entire time at Virginia Tech. In addition, I would like to express my gratitude to my "second family", The Browns, for their encouragement over the past 5 years. Miss Christy Brown, thanks for everything: support, encouragement, assurance, motivation, the list goes on and on…

Finally, I would like to thank the almighty God for providing me with the patience and endurance necessary to complete my journey (roller coaster so to speak) known as Virginia Tech. Without you neither the Appomattox River nor I would exist.

In search of a bigger and more exciting roller coaster…

Drew Hammond
Blacksburg, VA

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1.0 Introduction

A model is a tool that serves as a representation of something inherently complex. For example, architects construct scaled-down versions of proposed structures in order to give clients a visual representation of the completed project. A United States Geological Survey (USGS) 7.5-minute quadrangle is a paper representation of the complex terrain shown on the topographic sheet. Environmental engineers have developed a system of equations that represent and predict suspended solids concentrations within the settling basin of a water treatment plant.

With regard to tidal estuaries, engineers and hydrologists use hydrodynamic models to predict outputs, such as water surface elevations and velocities, given specific inputs, such as streamflows. In addition, they make use of water quality models to predict contaminant concentrations given hydrodynamics and contaminant loading rates. The hydrodynamic and water quality models utilized consist of a detailed set of equations that serve to represent complex physical processes. However, as the number of required equations to describe the processes in question increases, the computational time and model complexity also increases. As a result, numerical models have been developed to aid in the solution of complex process equations.

Computer models for simulating estuary hydrodynamics and water quality have existed for more than 30 years. Significant improvements have been made to the original computer models, therefore, improving the quality of model outputs. Today's computer models allow users to simulate in one, two, and three dimensions. In addition, they enable users to model waterbodies that are either steady state or dynamic systems. Model solution techniques have also been improved and the two most commonly employed are finite differences or finite elements. As a result of these improvements, users are now applying computer models to larger and larger estuary systems, such as the Chesapeake Bay, in order to estimate hydrodynamics and, more importantly, water quality.

Due to significant environmental degradation, Congress passed the Clean Water Act of 1972 and the Safe Drinking Water Act of 1974. The Clean Water Act of 1972 has command over the water quality in estuaries, reservoirs, lakes, rivers, streams, and wetlands. Even though the Clean Water Act has been in existence for approximately 30 years, there are still a significant number of impaired streams, rivers, and estuaries in the United States. For example, the Virginia Department of Environmental Quality (VADEQ) has listed portions of the following waterbodies as impaired because they violate current water quality standards: Appomattox River, James River, Maury River, New River, and the York River to name a few. In order to help improve the water quality in each of the impaired segments, computer models will be utilized to predict hydrodynamics and contaminant concentrations based upon specific model inputs.

The Appomattox River watershed is part of the James River basin, located in central Virginia, with an outlet in Hopewell, Virginia. The watershed drainage area is approximately 4146 km^2 (1600 mi^2) and encompasses 10 counties and 3 major cities. Landuse consists of forests and agricultural fields in the upper reaches of the watershed, whereas, the lower portion is mainly residential and commercial. Portions of the Appomattox River have been listed as impaired by USEPA due to high bacteria concentrations. One impaired segment of interest is the lower Appomattox River. This river segment is approximately 16.9 km (10.5 mi) long and passes through the cities of Colonial Heights, Petersburg, and Hopewell (VADEQ, 2002). Due to the tidal influence, the lower Appomattox River is an ideal study area for research on model implementation and the prediction of hydrodynamics and water quality in tidally influenced areas.

In order to advance the process of improving water quality assessment techniques within the lower Appomattox River, a computer model or models will be necessary to estimate river hydrodynamics and contaminant concentrations. However, since the model study area is tidally influenced, the model utilized will have to take into consideration the impacts of the flood and ebb tides that occur multiple times a day. In addition, the model should be fairly straightforward in terms of setup, and the computational time should not be excessive while using a current desktop computer. The model should be able to simulate a dynamic system, and it should employ a robust numerical solution technique, such as finite elements or finite differences.

After examining many candidate models, the research team selected the Dynamic Estuary Model (DYNHYD5) and the Water Quality Analysis Simulation Program (WASP6.1) (both by USEPA) to simulate hydrodynamics and water quality in the tidal portion of the Appomattox River. Model parameters were estimated from existing and newly collected datasets during initial setup. A calibration time period was used to modify and refine the model parameters. The models were then executed for a validation period, which differed from the calibration time frame to verify the validity of model parameters.

1.1 Problem Statement

The process to improve water quality in the lower Appomattox River can be advanced through the development and implementation of a computer-based hydrodynamic and water quality model. Readily available datasets from Hydrologic Simulation Program – Fortran (HSPF) simulation runs will provide a large majority of the required model inputs. To effectively implement computer models one must first understand the equations utilized in developing the specific model. These equations include the fundamental concepts of conservation of mass, conservation of energy, and mass balance. In addition, one must have a comprehension of the model solution method used, whether the technique is finite differences or finite elements. After model implementation one must also investigate suggested improvements to the modeling study. This includes determining enhancements to the currently utilized model as well as investigating the use of other models, which may provide more useful results.

1.2 Research Objectives

The main objective of this research is to advance the analytical process by which various proposals for improving water quality in the lower Appomattox River can be examined. A secondary objective is to investigate the possible use of multiple models to estimate estuary hydrodynamics and water quality. In order to meet these goals, the following tasks must be achieved:

- Examine an array of candidate estuary hydrodynamic and water quality models.
- Select and implement a hydrodynamic and water quality model utilizing existing datasets.
- Make use of streamflows and contaminant loadings from HSPF simulation runs as inputs to the hydrodynamic and water quality models.
- Compare the results of the hydrodynamic and water quality models to observed values for calibration and validation time periods.
- Investigate the possible use of other models for simulating estuary hydrodynamics and water quality, as well as determine their required inputs and solution techniques.

The successful completion of these objectives will produce a literature review detailing the historical uses of hydrodynamic and water quality models, the equations and theories used in 1-, 2-, and 3-dimensional modeling, and a discussion of numerical solution techniques. Hydrodynamic and water quality model matrices will be developed to aid in the selection of a model or models to be used for this research. A calibrated and validated hydrodynamic and water quality model will be produced to assist in improving water quality within the tidal Appomattox River.

The remaining portion of this document presents the necessary steps taken to complete these research objectives and the results obtained. Chapter 2 presents a detailed literature review and discusses the historical use of hydrodynamic models and water quality models. In addition, Chapter 2 provides a review of the applicable and available hydrodynamic and water quality models. Chapter 3 presents model theory, equations, and required inputs utilized in achieving the research objectives. Chapter 4 discusses the development and implementation of a hydrodynamic and water quality model for the lower Appomattox River. Chapter 5 communicates the results of the modeling study. Chapter 6 summarizes the modeling results and investigates the possible use of other models to obtain further estimates of hydrodynamics and water quality. Chapter 6 also develops areas of future research in tidal estuary hydrodynamic and water quality modeling.

2.0 Literature Review and Background Information

Chapter 2 presents historical uses of hydrodynamic and water-quality models, provides a review of the literature, and discusses the selection of a hydrodynamic and water quality model to be used for this research.

2.1 Historical Development of Hydrodynamic Models

Hydrodynamics models of rivers and estuaries have been in existence for more than 100 years. In 1875, a French engineer named Louis Fargue developed a physical model of the Garonne River near Bordeaux, France. Fargue used his model to perform 21 simulation runs during the course of 2 years, 1875 through 1876. In 1894, he published his results in an article entitled "Expériences relatives à l'action de l'eau courante sur un fond de sable" (Fargue, 1894) or "Experiments relating to the action of running water on a sand bottom." In so doing, Fargue achieved 2 goals. First, he verified the results of his 1868 research (Fargue, 1868) concerning the correlation between the configuration of the bed and the depth of water in the rivers. Second, he became the first engineer/scientist to use a hydraulic model in the discipline of river engineering (Hager, 2003). Shortly after Fargue, Osbourne Reynolds, whose name is synonymous with the term "Reynolds Number," constructed a physical model of the Mersery Estuary located near Liverpool, England.

As time passed and larger-scale estuaries were studied, the physical models utilized became larger and larger as well as more elaborate. Large riverine and estuarine models brought rise to laboratory facilities of enormous size to facilitate their operation. Even though present day physical models have become highly sophisticated, researchers must still contend with laboratory and scale effects. As a result, computer-based numerical models were developed to perform riverine and estuarine simulations. In addition, they have the capability to perform long term simulations for very large estuaries. Thus, enabling them to execute simulations more efficiently and more cost effectively than physical models (ASCE, 2000).

As noted in chapter 1, computer-based hydrodynamic models have been in existence for over 30 years. During the 1960's the USGS developed an implicit finite-difference model that would solve the 1-dimensional equations of motion or Saint Venant equations. One test location for the model was Three-Mile Slough, which is a 4.8 km (3mi) long man made channel located in a tide-influenced delta northeast of San Francisco, California. The second test location was a 9.15 km (5.7 mi) section of the Delaware River near Philadelphia, Pennsylvania. At this location the river is tidally influenced and the channel geometry is highly irregular. The USGS achieved fairly accurate results with their implicit finite-difference model and the development of other computer-based numerical models soon followed (Miller and Cunge, 1975). One hydrodynamic model developed and refined shortly after is USEPA's Dynamic Estuary Model (DYNHYD).

In 1970 Feigner and Harris (1970) released the Dynamic Estuary Model. This model was updated by Roesch et al. (1979) and became known as the Potomac Estuary

Hydrodynamic Model or DYNHYD2. Since 1979 DYNHYD2 has been enhanced and updated (Ambrose et al., 1988). The current release is DYNHYD5 (Ambrose et al., 1993a), which is distributed with USEPA's Water Quality Analysis Simulation Program (WASP) modeling software.

During the past 3 decades there have been a significant number of other computer-based hydrodynamic models developed besides the DYNHYD software. However, all of the models along with significant model developments and efforts cannot be discussed in detail. Table 2.1 below serves as an abbreviated list of other hydrodynamic models with references to model development and usage.

Table 2.1 Abbreviated List of Hydrodynamic Models with References

Model Name	References
River Hydrodynamics Model (RIVMOD-H)	Hosseinipour and Martin, 1992
Environmental Fluid Dynamics Code (EFDC)	Hamrick, 1992 Hamrick, 1996
Curvilinear Hydrodynamics in 3-Dimensions - Waterways Experiment Station (CH3D-WES)	Chapman et al., 1996

2.2 Historical Development of Water Quality Models

As noted by Lung (1993), the development of computer-based water quality models has closely followed water pollution control in the United States. Before 1970 the focus of water pollution control was directed towards achieving the ambient water quality standards. These standards were extremely hard to administer due to the fact that current biochemical oxygen demand (BOD) and dissolved oxygen (DO) models were not prepared for the challenge of translating the ambient standards to effluent discharge limits. In 1970 the USEPA was established and two years later Congress passed the Clean Water Act of 1972. Also, the National Pollutant Discharge Elimination System (NPDES) was developed by USEPA in 1972. As a result of this chain of events, computer-based numerical eutrophication and hydrothermal models were developed. For example, Orlob and Selna (1970) developed a mathematical model to simulate temperature distributions in the Fontana Reservoir, which is operated and maintained by the Tennessee Valley Authority (TVA). Additionally, Markofsky and Harleman (1973) worked to develop a mathematical model to predict dissolved oxygen concentrations as well as temperature variations in the same reservoir. A number of other changes soon followed, sparking the development of even more water quality models.

In 1977 water quality criteria were established for toxic substances, producing a need for water quality models to simulate toxics. In 1982 USEPA proposed the use of water quality-based controls instead of the conventional NPDES (technology-based) controls. As a result, wasteload allocation (point source) models were developed. In addition, USEPA established Superfund to initiate the clean up of the nation's hazardous waste sites. In turn, this sparked the development of computer-based sediment models. More recently, USEPA has turned its attention to a more comprehensive approach in cleaning up and protecting the U. S. waterbodies. The total maximum daily load (TMDL) process is explained in detail in Section 130.7 of the Clean Water Act. It is comprehensive in the fact that is considers wasteload allocations (point sources), load allocations (nonpoint sources), wildlife, and a margin of safety. As a result of the TMDL process, a significant number of new computer-based water quality models have been developed and implemented (Lung, 1993). One water quality model developed and refined throughout the process is USEPA's Water Quality Analysis Simulation Program (WASP).

In 1983 Di Toro et al. (1983) developed the first complete version of USEPA's Water Quality Analysis Simulation Program. Connolly and Winfield (1984) enhanced the modeling software the following year. Ambrose et al. (1988) updated the software once again and it became known as WASP4. Ambrose et al. (1993b) refined the modeling software, therefore, effectively producing WASP5. The current release is WASP6.1 (Wool et al., 2003) and is distributed and maintained by USEPA's Watershed and Water Quality Modeling Technical Support Center located in Athens, Georgia.

In addition to WASP, there are a significant number of computer-based water quality models that have been developed over the past 3 decades. However, all of the water quality models cannot be discussed in detail. Table 2.2 serves as an abbreviated list of other water quality models with references to model development and usage.

Table 2.2 Abbreviated List of Water Quality Models with References

Model	References
Enhanced Stream Water Quality Model (QUAL2E)	Brown and Barnwell, 1987 USEPA, 1995
Three-Dimensional Hydrodynamic-Eutrophication Model (HEM-3D)	Park et al., 1995 Sisson et al., 1997
Tidal Prism Water Quality Model (TPWQM)	Kuo and Neilson, 1988 Kuo and Park, 1994 Kuo et al., 1999 Shen et al., 2002
Two-Dimensional, Laterally-Averaged Hydrodynamic and Water Quality Model (CE-QUAL-W2)	Cole and Wells, 2002
Three-Dimensional Eutrophication Model (CE-QUAL-ICM)	Cerco and Cole, 1994 Cerco and Cole, 1995

2.3 Fundamental Equations of Motion

Improvements in numerical modeling have provided engineers and hydrologists the ability to simulate estuary hydrodynamics and water quality with the aid of their desktop computers. Computer-based hydrodynamic models predict outputs, such as in-stream velocities and water surface elevations, given specific inputs, such as streamflows. The same applies for computer-based water quality models. They simulate in-stream pollutant concentrations given water surface elevations, velocities, and pollutant loading rates.

Today's computer-based models allow the engineer or hydrologist to perform simulations in 3 dimensions (x, y, and z directions). With regards to hydrodynamics, modelers have the capability of simulating in-stream velocities in the longitudinal (x-direction), lateral (y-direction), and vertical (z-direction) directions. Therefore, if required, one can predict velocities associated with flow moving the length of the river, velocities associated with flow moving from the center of the river to the banks or vice versa, and velocities associated with flow moving from the river bed to the water surface or vice versa. In addition, the same principles apply to current water quality models. Engineers and hydrologists have the tools necessary to simulate changing pollutant concentrations in 3 dimensions.

The main concern today is whether or not to implement a 3-dimensional model if a 2-dimensional or 1-dimensional model will provide the same or similar results. This concern is partially due to the fact that the data requirements for a 3-dimensional model are extensive. In addition, the time and money required to setup, calibrate, and validate a 3-dimensional model are greater than those necessary for 2- and 1-dimensional models, especially if no data is present at the beginning of the process.

In order to gain a better understanding of model set up and implementation one must understand the equations utilized within the model. As a result, the equations for simulating estuary hydrodynamics (velocities and water surface elevations) are presented and briefly discussed below.

2.3.1 1-Dimensional Equations of Motion

One-dimensional estuary models provide engineers and hydrologists the capability of simulating hydrodynamics in the longitudinal direction or along the length of the estuary. They typically require less time and resources to set up, calibrate, and validate than equivalent 2- or 3-dimensional models. Due to their longitudinal environment, 1-dimensional models are best suited for estuaries that are long, narrow, and shallow in nature.

One-dimensional models employ the use of the conservation of mass and momentum equations to determine a number of estuary hydraulic characteristics, such as flowrates, depths, velocities, top widths, and cross-sectional areas (Martin and McCutcheon, 1999). Typically it is assumed that the density of water remains constant, therefore, the conservation of mass equation simplifies to the continuity equation. Considering the control volume shown in Figure 12-1 on page 280 (Chaudhry, 1993), the continuity equation (2.1) can be written:

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = q_L \qquad 2.1$$

Where $\frac{\partial A}{\partial t}$ is change in wetted channel cross-sectional area per unit time, $\frac{\partial Q}{\partial x}$ is the change in channel inflow or outflow per unit channel length, and q_L is the channel lateral inflow or outflow per unit channel length.

Chaudhry (1993) notes that for a channel with a regular cross-section, the top width (B) is a continuous function of depth (y) and presents a modified version of the continuity equation (2.2):

$$B\frac{\partial y}{\partial t} + \frac{\partial Q}{\partial x} = q_L \qquad 2.2$$

It is then noted that $\mathrm{Q} = \mathrm{AU}$, $\frac{\partial A}{\partial x} = B\frac{\partial y}{\partial x}$, and the equivalent channel depth (D) can be defined as $D = \frac{A}{B}$. This is substituted into equation 2.2 to yield:

$$\frac{\partial \mathrm{y}}{\partial \mathrm{t}} + \mathrm{D}\frac{\partial \mathrm{U}}{\partial \mathrm{x}} + \mathrm{U}\frac{\partial \mathrm{y}}{\partial \mathrm{x}} - \frac{\mathrm{q_L}}{\mathrm{B}} = 0 \qquad 2.3$$

Where $\frac{\partial y}{\partial t}$ is the change in depth per unit time, $\frac{\partial \mathrm{U}}{\partial \mathrm{x}}$ is the change in average cross-sectional velocity per unit channel length, and $\frac{\partial y}{\partial x}$ is the change in depth per unit channel length. A more detailed derivation can be seen on pages 279 and 280 of Chaudhry (1993).

For most 1-dimensional estuary models, the lateral inflow or outflow per unit channel length is assumed to be negligible when compared to the main channel inflows or outflows. As a result, the q_L term in equation 2.3 is zeroed out, therefore producing the Saint Venant continuity equation (2.4):

$$\frac{\partial \mathrm{y}}{\partial \mathrm{t}} + \mathrm{U}\frac{\partial \mathrm{y}}{\partial \mathrm{x}} + \mathrm{y}\frac{\partial \mathrm{U}}{\partial \mathrm{x}} = 0 \qquad 2.4$$

To reproduce the 1-dimensional momentum equation, one must apply Newton's second law, which states that the sum of the forces acting on a control volume is equal to the rate of change of momentum. Considering the control volume in Figure 12-2 on page 282 (Chaudhry, 1993), the momentum equation (2.5) can be written:

$$\sum \mathrm{F} = \frac{\mathrm{d}}{\mathrm{dt}}\int_{\mathrm{x_1}}^{\mathrm{x_2}} \mathrm{U\rho A dx} = \mathrm{U_2 \rho A_2 U_2} - \mathrm{U_1 \rho A_1 U_1} - \mathrm{V_x \rho q_L (x_2 - x_1)} \qquad 2.5$$

Where V_x is the velocity of the lateral inflow or outflow per unit channel length in the x-direction.

After manipulation, the momentum equation (2.5) simplifies to the following equation:

$$\frac{\partial Q}{\partial t}+\frac{\partial (QU)}{\partial x}+gA\frac{\partial y}{\partial x}=V_x q_L+gA(S_o-S_f) \qquad 2.6$$

Where S_o is the bed slope of the control volume, and S_f is the energy slope of the control volume.

Assuming that the lateral inflow or outflow per unit channel length (q_L) is approximately zero, equation 2.6 produces the well-known dynamic equation:

$$\frac{\partial U}{\partial t}+g\frac{\partial}{\partial x}\left(\frac{U^2}{2g}+y\right)=g(S_o-S_f) \qquad 2.7$$

The Saint Venant momentum equation (2.8) can be obtained from the dynamic equation (2.7) with further manipulation:

$$\frac{1}{g}\frac{\partial U}{\partial t}+\frac{U}{g}\frac{\partial U}{\partial x}+\frac{\partial y}{\partial x}=S_o-S_f \qquad 2.8$$

A more detailed derivation can be seen on pages 281 through 283 in Chaudhry (1993). Equations 2.4 and 2.8 are used to describe 1-dimensional open channel flow neglecting lateral inflows or outflows. With given initial and boundary conditions, one can solve the equations simultaneously to obtain velocity (U) and depth (y) at any distance (x) along the estuary at any time (t).

2.3.2 2-Dimensional Equations of Motion

Two-dimensional estuary models provide users the capability of simulating hydrodynamics in the longitudinal direction as well as the lateral direction or vertical direction. Depth averaged 2-dimensional models (simulation in the longitudinal and lateral directions) are employed when changes in the vertical direction are negligible, such as a completely mixed waterbody. They are typically applied to rivers, lakes, reservoirs, and estuaries that are long, wide, and relatively shallow. Laterally averaged 2-dimensional models (simulation in the longitudinal and vertical directions) are used when changes in the lateral (perpendicular to the main direction of flow) direction are negligible, such as a narrow stratified reservoir. They are normally applied to waterbodies that are long, narrow, and fairly deep (Martin and McCutcheon, 1999).

Additionally, 2-dimensional estuary models typically require more time and resources to setup, calibrate, and validate than 1-dimensional models. However, modeling in 2 dimensions provides the ability to unmask hydrodynamic changes in either the lateral or vertical direction that would not be available with a 1-dimensional model. Therefore, the results obtained from the hydrodynamic model may outweigh, in certain situations, the time, effort, and resources required for model setup and calibration.

2-dimensional, depth-averaged flow:

For 2-dimensional, incompressible, depth averaged flow the continuity equation (2.9) is given by Montes (1998):

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0 \qquad 2.9$$

Where $\frac{\partial u}{\partial x}$ is the change in the longitudinal velocity component per unit channel length, and $\frac{\partial v}{\partial y}$ is the change in the lateral velocity component per unit channel width.

The equations of momentum (2.10 and 2.11) for the corresponding flow regime are provided by Rahman (1988):

Longitudinal (x) direction:

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}=-\frac{1}{\rho}\frac{\partial P}{\partial x}+X+\upsilon\nabla^2 u \qquad 2.10$$

Lateral (y) direction:

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}=-\frac{1}{\rho}\frac{\partial P}{\partial y}+Y+\upsilon\nabla^2 v \qquad 2.11$$

where:
u = velocity in the longitudinal direction,
v = velocity in the lateral direction,
X = body force per unit mass in longitudinal direction,
Y = body force per unit mass in lateral direction,
P = pressure
υ = kinematic viscosity, and
∇^2 = Laplacian transform = $\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}$.

2-Dimensional, laterally-averaged flow:

For 2-dimensional, incompressible, laterally averaged flow Rahman (1988) gives the continuity equation (2.12):

$$\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} = 0 \qquad 2.12$$

Where $\frac{\partial w}{\partial z}$ is the change in the vertical velocity component per unit channel depth.

The equations of momentum (2.13 and 2.14) for the corresponding flow regime are (Rahman, 1988):

Longitudinal (x) direction:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + w\frac{\partial u}{\partial z} = -\frac{1}{\rho}\frac{\partial P}{\partial x} + X + \upsilon\nabla^2 u \qquad 2.13$$

Vertical (z) direction:

$$\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x} + w\frac{\partial w}{\partial z} = -\frac{1}{\rho}\frac{\partial P}{\partial z} + Z + \upsilon\nabla^2 v \qquad 2.14$$

where:
w = velocity in the vertical direction,
Z = body force per unit mass in vertical direction, and
∇^2 = Laplacian transform = $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}$.

2.3.3 3-Dimensional Equations of Motion

Three-dimensional estuary models enable the engineer or hydrologist to simulate hydrodynamics in the longitudinal, lateral, and vertical directions. As a result, they can be applied to all flow situations (1-, 2-, and 3-dimensional) and generally produce fairly accurate results. Since there are no dimensional limitations, 3-dimensional models can be used to simulate hydrodynamics in waterbodies of all types. For instance, they can be used on long, narrow, and shallow rivers or on wide and deep reservoirs with varying water density in the vertical direction. However, the time, effort, and resources required to set up, calibrate, and validate 3-dimensional models is quite extensive as compared to 1- or 2-dimensional estuary models. Therefore, the engineer or hydrologist must make a judgement before model selection and implementation. The use of a 3-dimensional hydrodynamic model when it is not warranted could entail a substantial misuse of time and funds.

For 3-dimensional, incompressible flow Rahman (1988) and Martin and McCutcheon (1999) provide the continuity equation (2.15):

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0 \qquad 2.15$$

The equations of momentum for 3-dimensional flow are similar to those for 2-dimensional flow. The main difference between the two is that the 3-dimensional equations contain terms for all flow directions, which is shown in equations 2.16 through 2.18 (Rahman, 1988):

<u>Longitudinal (x) direction:</u>

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}=-\frac{1}{\rho}\frac{\partial P}{\partial x}+X+\upsilon\nabla^2 u \qquad 2.16$$

<u>Lateral (y) direction:</u>

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}=-\frac{1}{\rho}\frac{\partial P}{\partial y}+Y+\upsilon\nabla^2 v \qquad 2.17$$

<u>Vertical (z) direction:</u>

$$\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}=-\frac{1}{\rho}\frac{\partial P}{\partial z}+Z+\upsilon\nabla^2 w \qquad 2.18$$

where:
u = velocity in the longitudinal direction,
v = velocity in the lateral direction,
w = velocity in the vertical direction,
X = body force per unit mass in longitudinal direction,
Y = body force per unit mass in lateral direction,
Z = body force per unit mass in vertical direction,
P = pressure
υ = kinematic viscosity, and
∇^2 = Laplacian transform = $\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$.

It should be noted that the complete 3-dimensional equations of motion (2.15 through 2.18) could be simplified in order to represent 2-dimensional or 1-dimensional flow patterns. They are an extremely powerful set of equations that can be applied to a number of different waterbodies. However, a great deal of computing power is required to simultaneously solve a set of partial differential equations. As a result, a number of different solution (approximations) techniques have been developed and employed with the aid of personal computers. With regards to open-channel flow, the two most robust numerical solution schemes are finite differences and finite elements, which are discussed in the next section.

2.4 Numerical Solution Techniques

Hydrodynamic models are based upon the conservation of mass (or continuity since water is assumed to be incompressible) and conservation of momentum, which are expressed as a set of partial differential equations. See equations 2.15 through 2.18 for the complete equations of motion for a 3-dimensional, incompressible flow. In order to simultaneously solve the equations of motion a number of solution techniques have been developed. The two most robust solution techniques in the area of open-channel flow are finite differences and finite elements. These solution methods are easily implemented through the use of personal computers, and they provide fairly accurate approximations to the exact solution of the complete equations of motion. In order to gain a better understanding of the finite difference and finite element solution methods, one must investigate the theory and equations behind each technique.

2.4.1 Finite Difference Solution Method

The early pioneers of the finite difference solution techniques were Runge in 1908 and Richardson in 1913. Finite difference methods were first used to analyze heat diffusion as well as solve stress analysis problems (Montes, 1998). Since the early 1900s, finite differences have been applied to a number of different situations including open-channel flow. The Saint Venant equations are a set of nonlinear partial differential equations describing the conservation of mass and momentum for 1-dimensional, open-channel flow assuming lateral inflow is negligible. Since the Saint Venant equations are expressed as nonlinear partial differentials, a closed-form solution is only available for very simple cases. As a result, an approximate solution to the Saint Venant equations can be obtained using finite differences (Chaudhry, 1993).

The basic principle behind all finite difference solution methods is the substitution of finite differences for partial derivatives. With regards to open-channel flow and the Saint Venant equations, the partial derivatives for velocity (V) and depth (y) would be replaced by discrete differences to be evaluated at fixed intervals for distance (Δx) and time (Δt) (Montes, 1998).

Consider the finite difference grid depicted in Figure 14-1 on page 311 of Chaudhry (1993). The x-axis represents the independent variable distance (x) and the y-axis represents the independent variable time (t). Point i denotes the $i\Delta x$ grid point, and point (i+1) designates the $(i+1)\Delta x$ grid point. The same applies for the y-axis. Point k denotes the $k\Delta t$ grid point, and point (k+1) designates the $(k+1)\Delta t$ grid point. In addition, point k is specified as the known time level and point (k+1) is the unknown time level. Once the finite difference grid has been generated, calculations are performed to determine the dependent variables at each grid point. Therefore, the dependent variable flow depth (y) at point (i,k) is designated as y_i^k.

Typical finite difference grids have straight edges and square corners. In addition, most grids utilize uniform x- and y-axis spacing. Since most finite difference grids make use of parallel lines, error is introduced when simulating natural boundaries. As a result, grid spacing may have to be reduced near places of rapid variability to accurately and effectively represent the system.

There are two distinctly different finite difference solution techniques, the explicit and implicit finite difference solution method. Each of these general solution techniques has three different solution approximations, the forward, backward, and central finite-difference approximation. Figure 14-1, page 311 of Chaudhry (1993) depicts the dependent variable (f) as a function of the independent variable (x). The forward finite difference approximation replaces the slope of the tangent at B with the slope of the line BC. The backward finite difference approximation replaces the tangent slope with the slope of line AB, and the central finite difference approximation replaces the slope with the slope of line AC. Chaudhry (1993) notes that the central finite-difference approximation is the most accurate. This is due to the fact that it best approximates the slope of the tangent at B, which is shown in Figure 14-1.

2.4.1.1 Explicit finite differences (Chaudhry, 1993)

Explicit finite difference schemes utilize discrete differences for the dependent variables in terms of the known time level (k) for the partial derivatives. Considering Figures 14-1 and 14-2 on page 311 of Chaudhry (1993), assume that point B is at the known time level (k). The partial derivative $\frac{\partial f}{\partial x}$ at x or point (i,k) can be estimated utilizing the three different finite difference approximations (equations 2.19 through 2.21):

Forward: $$\frac{\partial f}{\partial x} = \frac{f_{i+1}^k - f_i^k}{\Delta x} \qquad 2.19$$

Backward: $$\frac{\partial f}{\partial x} = \frac{f_i^k - f_{i-1}^k}{\Delta x} \qquad 2.20$$

Central: $$\frac{\partial f}{\partial x} = \frac{f_{i+1}^k - f_{i-1}^k}{2\Delta x} \qquad 2.21$$

It should be noted that these equations can also be modified and applied to the partial derivative of the function (f) with respect to time (t), $\frac{\partial f}{\partial t}$. When the finite difference approximations for $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial t}$ are solved simultaneously, they produce a solution for the function (f) for each Δx and Δt combination located on the finite difference grid.

There are a number of different explicit finite difference solution schemes. They include the Diffusive scheme, MacCormack scheme, Lambda scheme, and the Gabutti scheme. Chaudhry (1993) summarizes the formulations, boundary conditions, stability, and solution procedures for each method on pages 313 through 324 of his text.

2.4.1.2 Implicit finite differences (Chaudhry, 1993)

Implicit finite difference schemes utilize discrete differences for the dependent variables in terms of the unknown time level (k+1) for the partial derivatives. The partial derivative $\frac{\partial f}{\partial x}$ at point (i,k) can be estimated utilizing the three different finite difference approximations (equations 2.22 through 2.24):

Forward:
$$\frac{\partial f}{\partial x} = \frac{f_{i+1}^{k+1} - f_{i}^{k+1}}{\Delta x} \qquad 2.22$$

Backward:
$$\frac{\partial f}{\partial x} = \frac{f_{i}^{k+1} - f_{i-1}^{k+1}}{\Delta x} \qquad 2.23$$

Central:
$$\frac{\partial f}{\partial x} = \frac{f_{i+1}^{k+1} - f_{i-1}^{k+1}}{2\Delta x} \qquad 2.24$$

There are a number of varying solution schemes for implicit finite differences. They include the Preissmann scheme, Beam and Warming scheme, and Vasiliev scheme. The formulations, boundary conditions, stability, and solution procedures for each solution method are presented on pages 324 through 330 in Chaudhry (1993).

It should be noted that equations 2.19 through 2.24 present the approximation of partial differential equations utilizing two finite difference grid points. Solution techniques have been developed that utilize three or more grid points for performing approximations. These solution techniques are beyond the scope of this research.

2.4.2 Finite Element Solution Method

Finite elements provide a second solution technique to the same partial differential equations presented earlier in this chapter. However, the finite element solution method is a newer technique, which has not been used as extensively as finite differences.

There are a number of advantages for using finite elements in 2- or 3-dimensional open-channel flow simulation. As noted by Chaudhry (1993) and Jiang (1998), finite elements provide model users with the ability to perform simulations on irregular geometries.

Therefore, they can be applied to rivers and estuaries with complex natural boundaries without the additional grid refinements required by finite difference methods. In addition, finite elements can be organized anywhere in the estuary domain. Therefore, grid refinements with finite elements are typically easier to perform than those performed when using finite differences (Jiang, 1998). As a result, finite elements may prove to be more accurate and efficient in the solution of 2- and 3-dimensional open-channel flow problems with irregular boundaries.

The 1-, 2-, and 3-dimensional equations of motion for open-channel flow are nonlinear partial differential equations. As a result, some of the most complicated finite element methods must be employed to reach a solution. The main steps used in finite element analysis are (Kaliakin, 2002):

1. Domain discretization. The model domain (Ω) is arranged into a grid of elements and nodes. A typical rectangular finite element mesh is shown in Figure 7.1(B) on page 154 of Wang and Anderson (1982). Element numbers are circled, and node numbers are not circled.

2. Equations for each element are determined and are assembled into a series of global equations that apply to the entire domain. This assembly process is based upon the fundamental concept of continuity. Element equations typically have the following form (2.25):

   $$K^{(e)}\hat{\phi}_n^{(e)} = f^{(e)} \qquad 2.25$$

   where:
   $K^{(e)}$ is the element coefficient matrix,
   $\hat{\phi}_n^{(e)}$ is nodal unknowns vector associated with the element, and
   $f^{(e)}$ is the nodal forces vector associated with the element.

   The element equation assembly process results in a series of global equations typically in the following form (2.26):

   $$K\hat{\phi}_n = f \qquad 2.26$$

   where:
   K is the global coefficient matrix,
   $\hat{\phi}_n$ is the total nodal unknowns vector associated with the model, and
   f is the total nodal forces vector associated with the model.

3. Nodal specifications (boundary conditions) are specified along the entire model boundary (Γ), along element boundary nodes, or at nodes contained within any element. When known values of the principal dependent variables are specified along the model boundary they are referred to as essential (Dirichlet) specifications.

Natural (Neumann) specifications refer to known gradient values of the principal dependent variables specified along the model boundary.

4. Due to their nonlinear nature, the global equations are solved utilizing an iterative process such as the Newton-Raphson method. The Newton-Raphson solution scheme is discussed in detail in chapter 6 of Chaudhry (1993). In addition, completeness and compatibility requirements must be satisfied before the finite element method will converge upon the correction solution.

Due to its ability to handle complex irregular boundaries, which is typically the case of rivers and estuaries, the finite element solution method may prove to be a more accurate representation of the model network over finite differences. However, due to the nonlinear nature of the 1-, 2-, and 3-dimensional equations of motion, the finite element method is harder to implement than the finite difference solution method. As a result, the capability of finite elements to represent irregular waterbody geometry has not yet been fully exploited.

2.5 Review of Available, Applicable Hydrodynamic and Water Quality Models

The following hydrodynamic and water quality models were taken into account and reviewed for this research. Hydrodynamic and water-quality model summary matrices were developed and are shown in Tables C.1 and C.2 in Appendix C. Table C.3 serves as a detailed extension of Table C.1 and was developed in order to identify previous USEPA modeling experience for each water quality and hydrodynamic model being reviewed. Below is a brief discussion of model formulation and implementation as well as model availability.

2.5.1 Water Quality Analysis Simulation Program (Wool et al., 2003)

WASP is an uncoupled, unsteady, continuous simulation, 3-dimensional water quality model for simulating contaminant fate and transport in river systems including tidal estuaries. The major components of WASP include EUTRO (sub-model for simulating conventional water quality constituents), TOXI (sub-model for simulating toxicants), HEAT (sub-model for simulating heat transport), and hydrodynamic model linkage capabilities. WASP uses finite differences to solve mass balance equations, contaminant kinetics equations, and transport equations at each simulation time step. Furthermore, the model is capable of automatic time stepping in order ensure model stability.

Data requirements for WASP can be quite extensive especially for highly complicated systems that include contaminant transport within river or estuary beds. However, the data requirements for simulating bacteria concentrations are limited, therefore, greatly simplifying the implementation of the WASP modeling system to this research. As shown in Table C.3, WASP has been successfully used in numerous USEPA water quality studies.

WASP6.1 is the most current version of the WASP modeling system. It is distributed and supported by USEPA's Watershed and Water Quality Modeling Technical Support Center located in Athens, Georgia. Since WASP6.1 is an uncoupled water quality model, a hydrodynamic model is needed to provide the estuary water volumes and velocities required for simulation. WASP6.1 is currently configured so that it can be linked to three hydrodynamic models. They include the Dynamic Estuary Model (DYNHYD5), River Hydrodynamics Model (RIVMOD-H), and Environmental Fluid Dynamics Code (EFDC). A brief discussion of these hydrodynamic models is below.

2.5.1.1 Dynamic Estuary Model (Ambrose et al., 1993a)

DYNHYD5 is an unsteady, uncoupled, continuous simulation, 1-dimensional hydrodynamic model for simulating water velocities, flows, volumes, and heads using a channel junction (link-node) approach. The model can be applied to river systems with moderate bed slopes as well as to tidally influenced estuaries. The major component of DYNHYD5 is the model input file, which contains all data required for model execution. The model uses a finite difference scheme to solve the 1-dimensional Saint Venant's equations of continuity and momentum for each time step, and the output data is typically averaged over a longer time step to be used by the water quality program.

Due to the channel-junction (link-node) modeling approach, the data requirements for model execution are not extensive. River geometry can be obtained from existing USGS topographic sheets or existing bathymetry data. In addition, model inflows and outflows can be determined with the aid of a watershed modeling program, such as Hydrologic Simulation Program – Fortran (HSPF).

DYNHYD5 is most recent version of the modeling software. It is distributed and supported by USEPA's Center for Exposure Assessment Modeling (CEAM) through the WASP5 modeling software. Additional model support is also provided through the Watershed and Water Quality Modeling Technical Support Center. Model availability and support as well as ease of implementation makes DYNHYD an excellent candidate for the hydrodynamic portion of this research.

2.5.1.2 River Hydrodynamics Model (Hosseinipour and Martin, 1992)

RIVMOD-H is an uncoupled, unsteady, continuous simulation, 1-dimensional riverine model that can be used to simulate hydrodynamics and sediment transport. In addition, the model is applicable to tidally influenced areas. RIVMOD-H solves the 1-dimensional equations of conservation of momentum and conservation of mass (Saint Venant's equations) using a finite difference solution technique. Model data requirements are similar to those of DYNHYD5, and all information required for model execution is contained within a single input file.

RIVMOD-H is not distributed with the WASP5 modeling software. A special request must be submitted to CEAM to obtain the model software. At the present time, the research team has obtained the RIVMOD-H user's manual, but the model software has not been secured, therefore, limiting the ability of using the model for this research.

2.5.1.3 Environmental Fluid Dynamics Code (Hamrick, 1992; Hamrick, 1996)

EFDC is an unsteady, continuous simulation, 3-dimensional model that can been used to simulate hydrodynamics and sediment transport in riverine systems. It has been applied to a number of different tidal estuaries including the James River, York River, and the Chesapeake Bay. In addition, EFDC has been used in a number of different USEPA water quality studies. This is shown in Table C.3

EFDC data requirements and processing are quite extensive. Thirty separate input files are required in order to perform model simulations. EFDC does not employ a link-node model structure; instead, it uses horizontal and vertical grids to represent changes in channel geometry. Currently, a WINDOWS based preprocessor is being developed to aid in model setup and implementation. Due to the amount of time required for model set up, EFDC may not be a viable candidate for the time frame of this research.

EFDC was developed at the Virginia Institute of Marine Science (VIMS), College of William and Mary, Gloucester Point, Virginia. The model is public domain software and can be obtained from the author, Dr. John Hamrick. In addition, EFDC is now distributed and supported by USEPA's Watershed and Water Quality Modeling Technical Support Center.

2.5.2 Enhanced Stream Water Quality Model (Brown and Barnwell, 1987; USEPA, 1995)

QUAL2E is a coupled, steady-state, 1-dimensional model that can be utilized to estimate hydrodynamics and water quality in estuaries that are assumed to be well mixed. The model uses a backward finite difference solution scheme to solve the equations of mass transport and reaction kinetics. Model hydrodynamics are determined by calculating a series of steady, non-uniform water surface profiles. Therefore, QUAL2E is only capable of modeling waterbodies that receive steady flow inputs. As a result, the model may not be feasible for this research if flow inputs are determined to be unsteady.

QUAL2E divides a river system into computational elements consisting of headwaters, junctions, and reaches. For each reach there are approximately 26 different input parameters that must be specified. Overall, the model requires roughly 100 separate input parameters. As a result, the data requirements for QUAL2E are highly extensive and model setup could be quite tedious and time consuming.

The current version of QUAL2E, denoted as QUAL2K, has been developed to run within a Microsoft WINDOWS environment. The model is distributed and supported by USEPA's Watershed Water Quality Modeling Technical Support Center. In addition, QUAL2E is still available for Internet download and use through CEAM.

2.5.3 Three-Dimensional Hydrodynamic-Eutrophication Model (Park et al., 1995; Sisson et al., 1997)

HEM-3D is a 3-dimensional, unsteady, continuous simulation model for simulating estuarine hydrodynamics and water quality. The major components of the modeling software are the hydrodynamic sub-model, eutrophication sub-model, and a suspended sediment sub-model. HEM-3D utilizes finite differences to solve the equations of mass balance and kinetics to arrive at a water quality solution. Model hydrodynamics are calculated using EFDC, which has been integrated into the HEM-3D modeling software. Data requirements are the same as EFDC except for the addition of input parameters to perform water quality simulations.

HEM-3D was developed at VIMS and has since been refined at Tetra Tech, Inc. located in Fairfax, Virginia. Model user's manuals have been obtained from VIMS; however, the availability of the complete modeling software is in question. Due to extensive data requirements and uncertainty of model availability, HEM-3D may not be a feasible option for this research.

2.5.4 Tidal Prism Water Quality Model (Kuo and Neilson, 1988; Kuo and Park, 1994; Shen et al., 2002)

TPWQM is a coupled, 1-dimensional hydrodynamic and water quality model used to simulate longitudinal (with direction of flow) contaminant concentrations during flood tide. TPWQM is best applied to tidal creeks and coastal embayments. The model utilizes a finite difference solution technique to solve the equations of conservation of mass and reaction kinetics.

TPWQM is a product of VIMS in Gloucester Point, Virginia. The current version of the software can be implemented through a WINDOWS graphical user's interface (GUI) with the aid of GIS software. The TPWQM software was obtained and was thoroughly evaluated for a series of VIMS provided examples. Due to the research team's lack of experience with the required GIS software, TPWQM may not be a reasonable choice for this research.

2.5.5 Two-Dimensional, Laterally-Averaged, Hydrodynamic and Water Quality Model (Cole and Wells, 2002)

CE-QUAL-W2 is a coupled, unsteady, continuous simulation, 2-dimensional, laterally averaged hydrodynamic and water quality model. Since the model is laterally averaged, it is best suited for waterbodies that are relatively long and narrow. It can be applied to lakes, reservoirs, rivers, and estuaries. CE-QUAL-W2 uses a finite difference solution technique to solve the 2-dimensional equations of continuity and momentum. In addition, three numerical transport schemes have been incorporated into the model for use with the water quality routines.

Data requirements and availability are not limiting factors in the implementation of CE-QUAL-W2. However, Cole and Wells (2003) stress the fact that "garbage in equals garbage out" when applying or implementing the model.

The United States Army Corps of Engineers Waterways Experiment Station (USACE-WES) developed CE-QUAL-W2. USACE-WES provides limited support for the model in addition to the technical support services offered by private corporations such as J. E. Edinger Associates, Inc. (www.jeeai.com). The current release of CE-QUAL-W2 (Version 3.12) was developed by USACE-WES in conjunction with Portland State University. Model software and documentation can be obtained through the Internet from Portland State University (www.cee.pdx.edu/w2/). In addition, a user's forum (http://dneiper.cee.pdx.edu/w2/) with frequently asked questions and model support has been established through Portland State University.

2.5.6 CE-QUAL-ICM Three Dimensional Eutrophication Model (Cerco and Cole, 1995)

CE-QUAL-ICM is an uncoupled, unsteady, continuous simulation, 3-dimensional water quality model developed to study and simulate eutrophication processes in the Chesapeake Bay. The model has also been used to perform water quality studies in California, Delaware, Florida, and New York. CE-QUAL-ICM uses a finite difference solution technique to solve the equations of conservation of mass, transport, and kinetics within a grid of cells or volumes. The model does not calculate hydrodynamics, therefore, a hydrodynamic model is required. One suggested hydrodynamic model for linkage is Curvilinear Hydrodynamics in 3-Dimensions – Waterways Experiment Station (CH3D-WES).

For extremely detailed simulations approximately 16 separate input files are required for model execution. Model pre- and postprocessors must be provided by the user, therefore, data processing, model setup and implementation may become tedious and cumbersome. Due to time considerations, CE-QUAL-ICM may not be feasible modeling software for this research.

CE-QUAL-ICM is distributed and supported by USACE-WES located in Vickburg, Mississippi. The modeling software is currently available for U. S. Army Corps of Engineers use only and has not been made available to the general public. As a result, the CE-QUAL-ICM was not selected for this research.

2.5.6.1 Curvilinear Hydrodynamics in 3-Dimensions – Waterways Experiment Station (Chapman et al., 1996)

CH3D-WES is a continuous simulation, unsteady, 3-dimensional model for simulating hydrodynamics, temperature, and salinity in rivers and estuaries. The model has been used to simulate hydrodynamics within the Chesapeake Bay, which were later used by CE-QUAL-ICM to simulate water quality conditions. CH3D-WES utilizes finite differences to solve the equations of motion, conservation of mass, and conservation of volume within a grid of discrete cells.

CH3D-WES users must provide pre- and postprocessors to prepare model input files for simulation and process output files for graphical or tabular presentation. As a result of this, model setup and implementation may be tedious and time consuming.

CH3D-WES was developed by USACE-WES, and it is only available for USACE use only. Since CH3D-WES is unavailable to the general public, and it was only suggested for use with CE-QUAL-ICM, the modeling software was not selected for this research project.

2.6 Hydrodynamic and Water Quality Model Selection

After carefully reviewing all of the compiled data, the research team recommends that WASP6.1 coupled with DYHHYD5 be used to model the fate and transport of fecal coliforms within the lower Appomattox River. The team's recommendation is based on the following arguments:

- WASP6.1 coupled with DYNHYD5 has sufficient hydrodynamic and water quality capability to model the fate and transport of fecal coliforms within tidal estuaries.

- WASP6.1 can be linked to Hydrologic Simulation Program – Fortran (HSPF) for watershed loading inputs.

- WASP6.1 and DYHHYD5 were both developed by USEPA and have been used extensively in order to perform USEPA water quality studies for tidal estuaries. This is reflected in Tables C.1 and C.3.

- WASP6.1 and DYNHYD5 along with extensive documentation are readily available from the USEPA website (www.epa.gov). Therefore, model availability and user support is not a critical issue.

- WASP6.1 and DYNHYD5 can be used for long-term simulation over many tidal cycles. Also, WASP6.1 can automatic time step in order to ensure model stability.

WASP6.1 and DYNHYD5 are well matched computationally to the needs of this research and to the physical characteristics of the lower Appomattox River system. Data input requirements, particularly channel bathymetry, also are compatible with the data currently available to this research.

2.7 Case Studies Utilizing DYNHYD and WASP Modeling Software

The original WASP modeling software released by Di Toro et al. (1983) consisted of 2 previously developed sub-models. They are TOXI, which is still used to simulate toxic substances and EUTRO, which is still used to simulate eutrophication. Thomann (1975) and Thomann et al. (1976) utilized EUTRO to simulate phytoplankton in Lake Ontario. Di Toro and Connolly (1980) simulated the water quality of Lake Erie, and Di Toro and Matystik (1980) estimated the water quality of Lake Huron. In addition, Thomann and Fitzpatrick (1982) simulated the eutrophication processes in the Potomac River estuary. Also, Ambrose (1987) used the WASP modeling software to simulate volatile organic compounds within the Delaware River estuary. These modeling studies effectively document the historical use of the WASP modeling software. In addition, there are a number of current case studies that have been performed utilizing the WASP modeling software coupled with DYNHYD.

2.7.1 Snohomish River Estuary – Total Maximum Daily Load (Butkus et al., 1999)

Butkus et al. (1999) has developed a DYNHYD and WASP model of the Snohomish River (partially tidal river located in Washington State) to facilitate the establishment of a TMDL study on DO. An existing calibrated and validated DYNHYD4 hydrodynamic model of the study site was updated to DYNHYD5 for this water quality study. The DYNHYD5 model was used to predict river hydrodynamics under steady state and tidally influenced flow conditions. DYNHYD5 output was then linked with EUTRO5 (eutrophication sub-model within WASP5) to simulate ammonia and dissolved oxygen concentrations along the length of the river. The WASP5 model was executed assuming steady state pollutant loadings under the influence of tidal flow conditions. The modeling work performed resulted in the successful development of a USEPA approved TMDL for the Snohomish River.

2.7.2 Watershed Based Simulation of Fecal Coliforms within the Back Bay of Biloxi (Renick, 2001)

Renick (2001) examined the simulation of fecal coliforms within the Back Bay of Biloxi, which feeds into Biloxi Bay and then into the Mississippi Sound. The study area utilized was approximately 1916 km^2 (740 mi^2) and included waterbodies both tidal and non-tidal. In addition, the study area was deemed to be a relatively narrow, long, and shallow embayment. As a result, the DYNHYD5 and WASP5 modeling software was chosen to simulate the fate and transport of fecal coliforms within the tidal reaches. As noted by the author, the hydrodynamic model utilized was calibrated and validated prior to this modeling study (Shindala et al., 1996). In addition, Shindala et al. (1996) developed a calibrated and validated EUTRO5 model of the study site to simulate nutrients, phytoplankton, and dissolved oxygen. These 2 models were used as a starting for this modeling study. A nonpoint source model (NPSM) was developed for the watershed utilizing USEPA's BASINS 2.0 software. The NPSM outputs were then used as inputs for the DYNHYD5 and EUTRO5 models. The models were then verified, and fecal coliform concentrations were simulated for a representative "wet" year and representative "dry" year.

2.7.3 Hydrodynamic and Water Quality Model for the Delaware Estuary (Delaware River Basin Commission, 2003)

The Delaware River Basin Commission (2003) developed a DYNHYD5 and WASP5 model of the Delaware Estuary (part is tidal) as part of a TMDL study on polychlorinated biphenyls (PCBs). A previous DYNHYD5 model of the estuary was updated in order to extend the simulated hydrodynamics and mass transport to the Atlantic Ocean. Tidal heights at various points along the estuary were used to calibrate the DYNHYD5 model. The final calibration of the model spans 577 days or September 1, 2001 to March 31, 2003. The calibrated outputs from DYNHYD5 were then linked with the TOXI5 (toxic substances) sub-model of WASP5. WASP5 was then used to simulate chloride concentrations within the estuary. Calibration of WASP5 was achieved by varying estuary dispersion coefficients and the water quality advection factor. After successfully reproducing estuary chloride concentrations then model was then deemed fit for simulating PCBs during the TMDL process.

3.0 Model Theory and Required Inputs

Chapter 3 introduces the model theory and required inputs utilized to support the research objectives presented in chapter 1. In summary, the research objectives are:

- Examine an array of candidate estuary hydrodynamic and water quality models.
- Select and implement a hydrodynamic and water quality model utilizing existing datasets.
- Make use of streamflows and contaminant loadings from HSPF simulation runs as inputs to the hydrodynamic and water quality models.
- Compare the results of the hydrodynamic and water quality models to previously observed values for predetermined calibration and validation time periods.
- Investigate the possible use of other models for simulating estuary hydrodynamics and water quality, as well as determined their required inputs and solution techniques.

DYNHYD5 is an unsteady, uncoupled, continuous simulation, 1-dimensional hydrodynamic model for simulating water velocities, flows, volumes, and heads using a channel junction (link-node) approach. The model uses a finite difference scheme to solve the 1-dimensional equations of continuity and momentum. Since DYNHYD5 is an uncoupled hydrodynamic model, a water quality model is required to simulate bacteria concentrations within the tidal Appomattox River. As a result, WASP6.1 was chosen as the water quality model to be used for this research.

WASP6.1 is an uncoupled, unsteady, continuous simulation, 3-dimensional water quality model for simulating contaminant (including bacteria) fate and transport in river systems including tidal estuaries. The model uses finite differences to solve the necessary mass balance equations, contaminant kinetics equations, and transport equations. Since WAPS6.1 is an uncoupled water quality model, required hydrodynamics are supplied by DYNHYD5 through the use of a hydrodynamic linkage file.

In order to perform hydrodynamic and water quality simulations of the tidal Appomattox River, DYNHYD and WASP made use of existing datasets as well as streamflows and contaminant loadings derived from previously performed HSPF simulation runs. Figure 3.1 serves as a representation of how DYNHYD, WASP, and HSPF were linked together in order to perform this research.

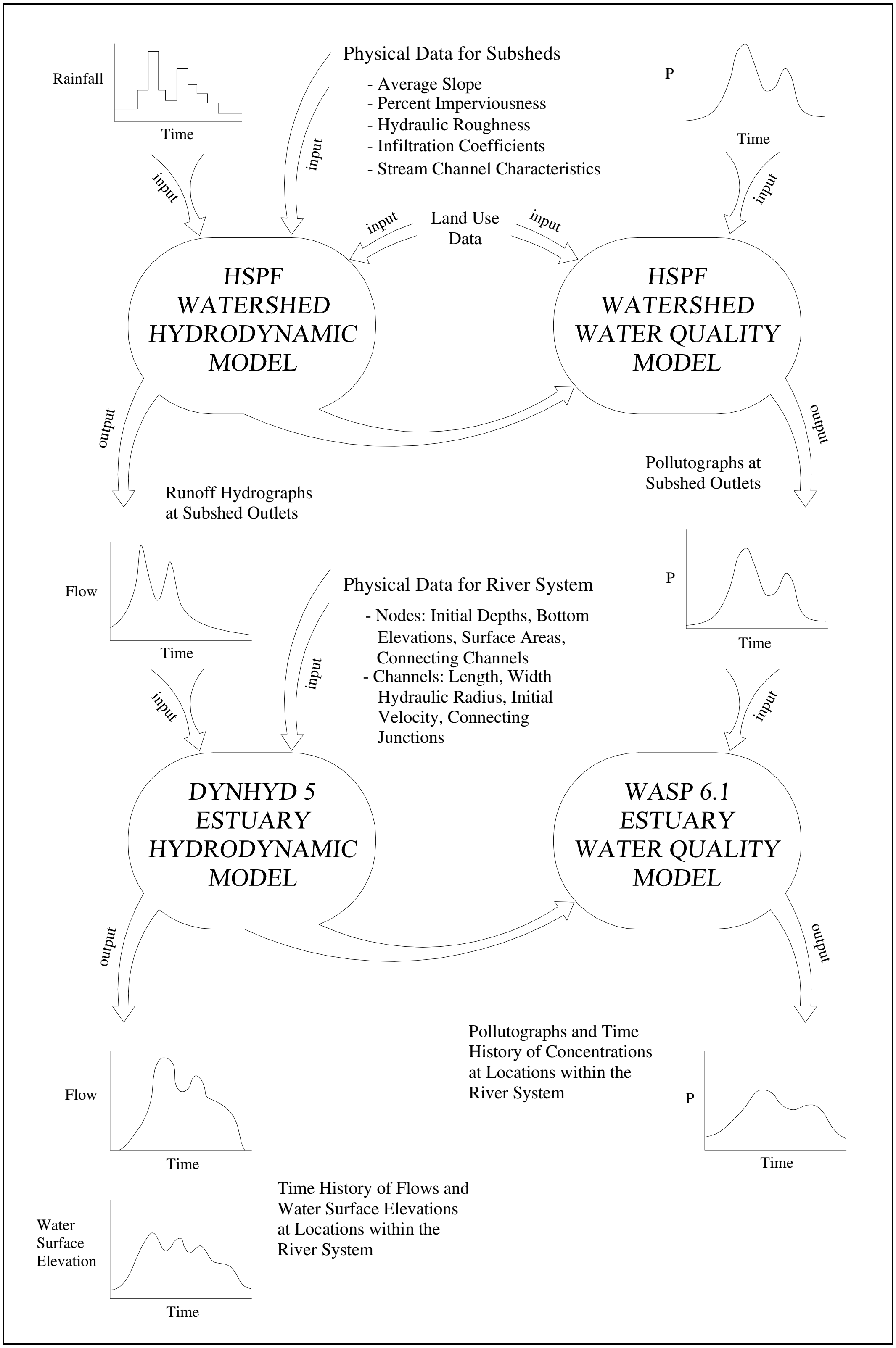

Figure 3.1 Model Linkage Representation

DYNHYD5 and WASP6.1 background theory and required model inputs are discussed. Section 3.1 develops the theories and equations used in the development of the DYNHYD5 hydrodynamic model. Also, it describes the required inputs of the hydrodynamic model. Section 3.2 discusses the theories and equations utilized in the development of the WASP6.1 water quality model. In addition, it examines the necessary model inputs.

3.1 DYNHYD5 Model Architecture

The principal DYNHYD5 equations and inputs are discussed to provide a more complete understanding of the model architecture. A typical DYNHYD5 model run consists of the model source code written in FORTRAN 77 and the input data file written in ASCII text. Since the input file is coded in ASCII format, it can be generated with a number of different software packages including the DYNHYD5 preprocessor, text editors, and spreadsheets.

DYNHYD5 utilizes a channel-junction (link-node) model network to perform simulations. Streams, rivers, or estuaries are broken down into a series of channels (links) and junctions (nodes). Figure 3.2 below serves as a visual representation of the link-node model network for a simple stream or river.

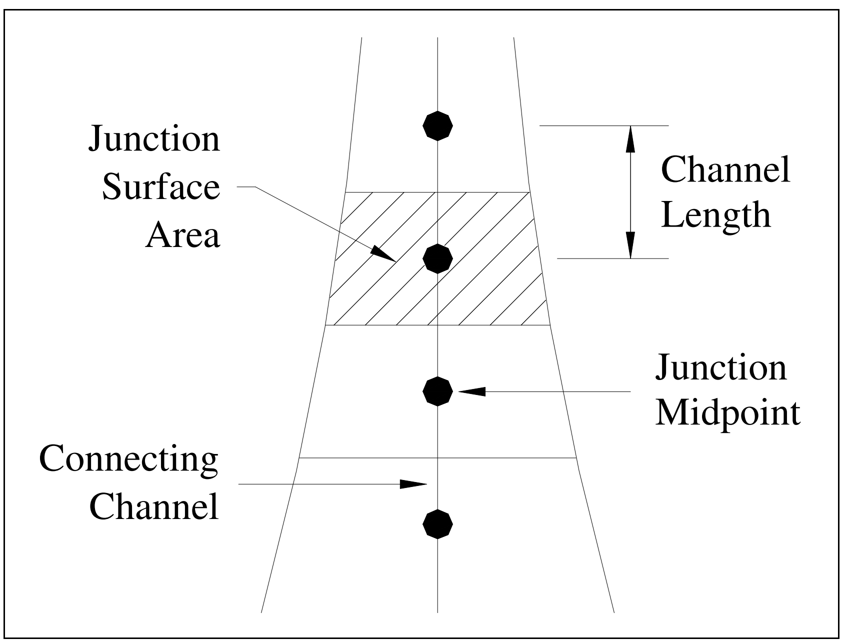

Figure 3.2 DYNHYD5 Link-Node Model Network
(Adapted from: Ambrose et. al, 1993a)

Each link serves to connect two junctions, one upstream and one downstream. In Figure 3.2, each junction is connected by an upstream and downstream link. However, DYNHYD5 has the capability of simulating complex branching river systems. The version of DYNHYD5 used for this research has the ability to simulate junctions with a maximum of 6 links either leaving or entering a single junction.

3.1.1 DYNHYD5 Model Equations (Ambrose et al., 1993a; Martin and McCutcheon, 1999)

The DYNHYD5 model network is arranged into a series of channels (links) and junctions (nodes) as previously discussed and shown in Figure 3.2. Conceptually, model junctions are volumetric units that receive and store water from their respective connecting channels. DYNHYD5 solves the 1-dimensional equation of continuity (3.1) at each junction assuming no lateral inflow, which is given by:

$$\frac{\partial A}{\partial t} = -\frac{\partial Q}{\partial x} \qquad 3.1$$

where:
A = cross-section area (m^2), and
Q = flowrate (m^3/s).

Further modifications to equation 3.1 are made following a few basic assumptions. DYNHYD5 assumes that the irregular cross-sectional areas of the junction connecting channels can be approximated by equivalent rectangular cross-sections. In addition, the model assumes that the channels have a constant width (B). As a result, the modified equation of continuity (3.2) is presented as:

$$\frac{\partial H}{\partial t} = -\frac{1}{B}\frac{\partial Q}{\partial x} \qquad 3.2$$

where:
H = water surface elevation or head (m),
B = channel width (m), and
Q = flowrate (m^3/s).

To solve equation 3.2, DYNHYD5 makes use of the finite difference solution technique discussed in chapter 2. The continuity equation (3.2) can be rewritten in finite difference form, which is shown in equation 3.3:

$$\frac{H_j^t - H_j^{t-1}}{\Delta t} = -\frac{\Delta Q_j}{B_j \Delta x_j} \qquad 3.3$$

where:
H_j^t = water surface elevation (m) for junction j at the current time step,
H_j^{t-1} = water surface elevation (m) for junction j at the previous time step,
Δt = time step (sec),
ΔQ = summation of inflows and outflows (m^3/s) for junction j,
B_j = mean width (m) of junction j, and
Δx_j = length (m) of junction j.

Equation 3.3 can be rewritten and expressed in finite difference form, which is the equation continuity equation DYNHYD5 solves at each junction (3.4):

$$H_j^t = H_j^{t-1} - \Delta t \frac{\sum Q_j}{A_j^s} \qquad 3.4$$

where:
Q_j = junction j inflow or outflow (m^3/s), and
$A_j^s = B_j \Delta x_j$ = surface area (m^2) of junction j.

Channels (links) are used in order to transport water between upstream and downstream junctions. Within each channel, DYNHYD5 solves the 1-dimesional conservation of momentum equation (3.5):

$$\frac{\partial U}{\partial t} = -U \frac{\partial U}{\partial x} + a_{g,\lambda} + a_f + a_{w,\lambda} \qquad 3.5$$

where:
U = longitudinal channel velocity (m/s),
t = time (sec),
x = longitudinal channel distance (m),
$a_{g,\lambda}$ = gravitational acceleration along longitudinal (λ) axis of channel (m/s^2),
a_f = frictional acceleration (m/s^2), and
$a_{w,\lambda}$ = wind acceleration along longitudinal (λ) axis of channel (m/s^2).

The gravitational, frictional, and wind acceleration terms are discussed and derived on pages 3 through 11 in Ambrose et al. (1993a). DYNHYD5 developers note that estuaries do not typically experience steady uniform flow; however, in the case of extremely small time steps the flow can be assumed to be uniform and steady. As a result, the frictional acceleration term is expressed as a function of the Manning's equation (3.6) for uniform, steady, flow:

$$U = \frac{1}{n} R^{2/3} S_f^{1/2} \qquad 3.6$$

where:
U = longitudinal channel velocity (m/s),
n = roughness coefficient,
R = hydraulic radius (equal to flow depth for wide rectangular channels), and
S_f = energy slope (m/m) = $\frac{\partial H}{\partial x}$.

Utilizing equation 3.6 and the derivations found on pages 3 through 11 in Ambrose et al. (1993a), the modified momentum equation (3.7) is expressed as:

$$\frac{\partial U}{\partial t} = -U\frac{\partial U}{\partial x} - g\frac{\partial H}{\partial x} - \frac{gn^2}{R^{4/3}}U|U| + \frac{C_d}{R}\frac{\rho_a}{\rho_w}W^2\cos\psi \qquad 3.7$$

where:
g = gravitational acceleration (9.81 m/s^2),
C_d = drag coefficient (unitless) and assumed to be 0.0026,
ρ_a = density of air (kg/m^3),
ρ_w = density of water (kg/m^3),
W = wind speed measured 10 meters above water surface (m/s), and
ψ = angle between wind direction and channel direction (degrees).

DYNHYD5 also uses finite differences to solve the momentum equation. As a result, equation 3.7 must be rewritten in finite difference form (3.8), with all terms on the right hand side of equation 3.8 referenced to the previous time step (t-1) or (t-Δt):

$$\frac{U_i^t - U_i^{t-1}}{\Delta t} = -U_i^{t-1}\frac{\Delta U_i}{\Delta x_i} - g\frac{\Delta H_i}{\Delta x_i} - \frac{gn_i^2}{R_i^{4/3}}U_i^{t-1}\left|U_i^{t-1}\right| + \frac{C_d}{R_i}\frac{\rho_a}{\rho_w}W_i^2\cos\psi_i \qquad 3.8$$

where:
U_i^t = velocity (m/s) in channel i at current time step,
U_i^{t-1} = velocity (m/s) in channel i at previous time step,
Δt = time step (sec),
$\frac{\Delta U_i}{\Delta x_i}$ = channel i velocity gradient (1/sec),
$\frac{\Delta H_i}{\Delta x_i}$ = channel i water surface gradient (m/m), and
i = channel number.

Utilizing the continuity equation (3.1), recognizing that Q = AU, and rearranging the terms yields the following velocity gradient (3.9):

$$\frac{\partial U}{\partial x} = -\frac{1}{A}\frac{\partial A}{\partial t} - \frac{U}{A}\frac{\partial A}{\partial x} \qquad 3.9$$

It should be noted that A = BR (for wide rectangular channels) and that ∂A = BΔH. Using these relationships, equation 3.9 can be rewritten in finite difference form:

$$\frac{\Delta U_i}{\Delta x_i} = -\frac{1}{R_i}\frac{\Delta H_i}{\Delta t} - \frac{U_i}{R_i}\frac{\Delta H_i}{\Delta x_i} \qquad 3.10$$

Where $\frac{\Delta H_i}{\Delta t}$ is the average water surface elevation change between the junctions upstream and downstream of channel i.

DYNHYD5 uses equation 3.10 in conjunction with equation 3.8 to solve the finite difference form of the momentum equation (3.11) for every channel in the model network. The finite difference form of the momentum equation is given as:

$$U_i^t = U_i^{t-1} + \Delta t\left[-U_i^{t-1}\frac{\Delta U_i}{\Delta x_i} - g\frac{\Delta H_i}{\Delta x_i} - \frac{gn_i^2}{R_i^{4/3}}U_i^{t-1}\left|U_i^{t-1}\right| + \frac{C_d}{R_i}\frac{\rho_a}{\rho_w}W_i^2\cos\psi_i \right] \qquad 3.11$$

Where $\frac{\Delta U_i}{\Delta x_i}$ is the velocity gradient of channel i, which is provided by equation 3.10.

DYNHYD5 utilizes a second-order Runge-Kutta finite difference technique to solve the continuity equation (3.4) within each junction and the momentum equation (3.11) within each channel (Martin and McCutcheon, 1999). The solution method is inherently explicit, and the discrete differences for the dependent variables are expressed in terms of the known time level (t-1), which is shown in equations 3.4 and 3.11. The second-order Runge-Kutta technique performs trial calculations at the midpoint (t + Δt/2) of the selected model time step. The results obtained at the midpoint are then used to compute values across the entire model time step (Δt) (Press et al., 1992). As a result, the second-order Runge-Kutta technique is classified as a central difference (midpoint) approximation. Explicit central difference techniques are developed in further detail in section 2.4.1.1 of chapter 2. Also, the eight step Runge-Kutta procedure that is employed by DYNHYD5 is outlined on page 21 of Ambrose et al. (1993a).

3.1.2 DYNHYD5 Required Inputs (Ambrose et al., 1993a)

As noted earlier, the DYNHYD5 input data file is coded in space-delimited ASCII text. As a result, the input file can be generated with a number of different software packages including the DYNHYD5 preprocessor, text editors, and spreadsheets. PREDYN, the DOS-based DYNHYD5 preprocessor, was used to generate the initial input data files for this research. After gaining significant experience with the structure of the input files, TextPad 4.7.2 (developed by Helios Software Solutions) was used to generate and edit the final DYNHYD5 input data files. The use of a text editor proved to be fast and efficient for input file manipulation when performing numerous hydrodynamic simulations.

A typical DYNHYD5 input data file is organized into 12 different groups, which are contained within a single ASCII file. The 12 groups include, but are not limited to simulation control, printout control, junction data, channel data, inflow data, wind data, and precipitation/evaporation data. The 12 data groups and their respective inputs are listed below. Sample DYNHYD5 input files used in this research are provided in

Appendix D. Readers are encouraged to review chapter 2 of Ambrose et al. (1993a) for a complete description of the DYNHYD5 input data file organization.

Group A: Simulation Control

Data group A contains information pertaining to the model simulation run. Parameters found within group A are the simulation title and simulation description. In addition, group A contains the number of junctions and channels within the model network, number of time steps within model execution, model time step, junction and channel initial conditions, as well as beginning and ending dates for model simulation.

Group B: Printout Control

Data group B consists of all of the information governing model printouts. Parameters that are found within group B include the beginning time for model printout, time step for model printout, and a list of junction numbers that the model will printout information for.

Group C: Hydraulic Summary

The hydraulic summary (group C) contains information pertaining to the storage of hydrodynamic results within a separate text file to be used later for water quality simulations. Parameters located within group C are the hydrodynamic scratch file options, beginning date for model results storage, intermediate results storage time interval, ratio of hydraulic time steps to one water quality time step, as well as the time interval to store results on a scratch file.

Group D: Junction Data

Group D consists of junction data for the entire model network. Junction parameters include junction number, water surface elevation at model start (referenced to a common model datum), junction surface area, junction bottom elevation (referenced to a common model datum), and channel numbers entering or existing the junction (limited to a maximum of 6 different channels). Each junction within the model network contains 1 space-delimited line with the aforementioned information.

Group E: Channel Data

Group E contains information pertaining to the channels found with in the model network. Channel parameters consist of channel number, channel length, channel width, channel hydraulic radius, channel direction (measured from north), channel roughness coefficient, initial velocity at model start, as well as upstream and downstream junction numbers. Each channel is described with 1 space-delimited line containing the previously discussed information.

Group F: Inflow Data

Group F consists of the model constant and variable inflow data. Constant inflow parameters are the number of inflows, junction number receiving the inflow, and the constant inflow value into the respective junction. Variable inflow parameters include the number of variable inflows, junction number receiving the variable inflow, the number of data points describing the variable inflow, simulation time of variable inflow data points, and values of variable inflow data points. Within the DYNHYD5 modeling network, inflow values are negative and outflow values are positive.

Group G: Seaward Boundary Data

Group G is used to describe model seaward boundaries if present. Three options exist in DYNHYD5 for simulating a seaward boundary. The first option allows the user to specify the tidal period, tidal input starting time, as well as the 7 regression coefficients for the following tidal regression equation (3.12):

$$y = A_1 + A_2 \sin(\omega t) + A_3 \sin(2\omega t) + A_4 \sin(3\omega t) + A_5 \cos(\omega t) + A_6 \cos(2\omega t) + A_7 \cos(3\omega t) \tag{3.12}$$

where:
y = elevation of tide below or above common model datum (m),
A_i = regression coefficient (m),
t = time (hr), and
$\omega = \dfrac{2\pi}{\text{Tidal} \cdot \text{Period}}$ (1/hr).

Option 2 enables the user to specify the tidal period, tidal input starting time, as well as tidal elevations and their respective times for a single tidal cycle. The model will utilize the data provided to determine the regression coefficients for equation 3.12. Option 3 allows the user to specify tidal elevations as well as their respective times for the entire simulation time period. If continuous records of water surface elevation have been taken with a tidal stage recorder then option 3 would provide the most accurate representation of the tidal cycle, especially if the tidal function is variable.

Group H: Wind Data

Group H contains the wind speeds and directions imposed upon the model throughout the simulation. Wind parameters include wind speed measured 10 meters above the water surface, wind direction measured in degrees from true north, total number of wind data points, as well as the day, hour, and minute of each observed wind data point.

Group I: Precipitation/Evaporation Input

Group I enables the user to specify a variable precipitation rate or evaporation rate, which is assumed to be uniform over the entire model surface area (total of all junction surface areas). Precipitation/evaporation input parameters include the total number of precipitation and/or evaporation data points, scale factor (used to increase or decrease the magnitude of precipitation/evaporation values), and a units conversion factor (used to ensure that the precipitation/evaporation rate has the correct units for simulation). In addition, group I parameters consist of variable precipitation/evaporation values (m/s) and the day, hour, and minute of each observed data point. Within the DYNHYD5 modeling framework, precipitation rates are positive values and evaporation rates are negative values.

Group J: Junction Geometry Input Data

Group J allows the user to specify whether or not model junctions have variable surface areas. Junction geometry parameters include the number of junctions with variable surface areas, junction number, as well as the rate of change in junction surface area with regards to junction water surface elevation.

Group K: Channel Geometry Input Data

Group K contains information pertaining to channels with varying widths with respect to water surface elevation. Channel geometry input parameters consist of the number of channels with varying widths, channel number, and the rate of change in channel width with regards to water surface elevation. If the rate of change in channel width is specified as zero then the channel is assumed to be rectangular in cross-section.

Group L: DYNHYD Junction to WASP Segment Map

Group L enables to user to specify which DYNHYD5 junctions will be mapped to the water quality model, WASP6.1. More specifically, there are 2 DYNHYD to WASP linkage options. Option 1 instructs DYNHYD5 to print out time-variable water surface elevations and velocities for mapped junctions. Option 2 directs DYNHYD5 to print out 1-set of water surface elevations and velocities for mapped junctions. This option should only be employed when changes in segment heads and velocities are negligible. WASP segment map parameters include the total number of DYNHYD5 junctions to map, junction number, as well as the junction's corresponding WASP6.1 segment number.

In order to generate a complete input file for a complex DYNHYD simulation, a significant amount of input data must be collected and processed. The data collection process can be extensive, exhausting, and time consuming. As a result, pre-existing datasets were utilized for this research when possible. Data collection and data processing performed to generate DYNHYD5 input files is discussed in detail in section 3.4 of this chapter.

3.1.3 DYNHYD5 Model Stability

Computational stability of the DYNHYD5 model is a function of the Courant-Friedrichs-Lewy stability criteria given by equation 3.13 (Martin and McCutcheon, 1999):

$$\Delta t \leq \frac{\Delta x}{C_d} \qquad 3.13$$

where:
Δt = simulation time step (sec),
Δx = channel length (m), and
C_d = dynamic wave celerity relative to the river bank (m/s).

Equation 3.13 can be rewritten in terms of channel length by expressing the dynamic wave celerity as a function of channel velocity and depth (Ambrose et al., 1993a):

$$L_i \geq \left(U_i \pm \sqrt{gY_i}\right)\Delta t \qquad 3.14$$

where:
L_i = length of channel i (m),
U_i = mean velocity within channel i (m/s),
g = gravitational acceleration (9.81 m/s^2),
Y_i = mean depth of channel i (m), and
Δt = time step (sec).

In order to ensure computational stability, all DYNHYD5 channels must be longer than the dynamic wave celerity multiplied by the model time step. Therefore, during model set up, the user must have an estimate of the mean channel velocity (Martin and McCutcheon, 1999).

3.1.4 Hydrodynamic Linkage File

In order to link DYNHYD5 hydrodynamics to WASP6.1 (water quality model), users must create an external hydrodynamic linkage file. This can be accomplished directly within the DYNHYD5 modeling framework. Within DYNHYD data group C (Hydraulic Summary) the user tells the model to create a permanent external hydrodynamic linkage file formatted for WASP6.1. In addition, the user specifies the starting day, hour, and minute for the linkage file. Next, the user specifies the time interval (typically 12.5, 24, or 25 hours) for storing intermediate DYNHYD5 results in a temporary scratch file. The ratio of hydrodynamic time steps per water quality time step is defined, which establishes the WASP6.1 simulation time step. However, these are only the initial steps in creating an external hydrodynamic linkage file. Examples of DYNHYD5 data group C inputs can be seen in the sample DYNHYD5 input files provided in Appendix D.

In addition, users must also create a map that relates DYNHYD5 junctions to WASP6.1 segments. This is accomplished through the use of DYNHYD5 data group L (DYNHYD Junction to Wasp Segment Map). Within this data group, the user has the capability of telling the model to write one set of segment depths and velocities for use by WASP6.1 or to write time-variable segment depths and velocities within the hydrodynamic linkage file. For this research, time-variable segment depths and velocities were written to the external linkage file. This option was chosen due to the fact that the model study area was tidally influenced and junction water surface elevations and channel velocities were constantly changing. Within data group L, the user must also map DYNHYD5 junctions to WASP6.1 segments. This is accomplished by specifying the DYNHYD5 junction number in one column and the corresponding WASP6.1 segment number in an adjacent column. It should be noted that DYNHYD5 boundary junctions are designated with a '0" in the WASP6.1 segment number column. Examples of DYNHYD5 data group L inputs can be seen in the sample DYNHYD5 input files provided in Appendix D.

After executing DYNHYD5, an external hydrodynamic linkage file (HYD file extension) is created in the same directory as the DYNHYD5 input file. The external hydrodynamic linkage file will contain WASP6.1 segment volumes at the beginning of each water-quality model time step. These volumes will be used by WASP6.1 in order to determine contaminant concentrations within each segment. In addition to segment volumes, the hydrodynamic linkage file will contain interfacial flows between adjacent segments that have been averaged over the water quality time step (assuming it is larger than the hydrodynamic model time step). These interfacial flows will be used by WASP6.1 to determine contaminant mass transport between connecting segments. For this research, the linkage file also contained time-variable segment depths and velocities. These parameters are typically used by WASP6.1 to calculate volatilization and reaeration rates within each segment (Ambrose et al, 1993a).

The size of the hydrodynamic linkage files can become rather large, depending on the length of the water quality simulation and the selected water quality time step. As a result, it is suggested that a personal computer with a rather larger hard drive be utilized when performing DYNHYD5 simulations where external linkage files are being created. This will eliminate the possibility of simulation stoppage due to lack of required hard drive space.

3.2 WASP6.1 Model Architecture and Required Inputs

The prevalent WASP6.1 equations and inputs are discussed to provide a more complete understanding of the model architecture. A typical WASP6.1 model run consists of the model source contained within Dynamic Link Libraries (DLLs), the input file generated using the WINDOWS based preprocessor, and the hydrodynamic linkage file prepared by DYNHYD5.

WASP6.1 utilizes a segmented model network to perform simulations, in which streams, rivers, or estuaries are broken down into a series of model segments. Figure 3.3 below provides a graphical representation of the segmented model network for a complex river system.

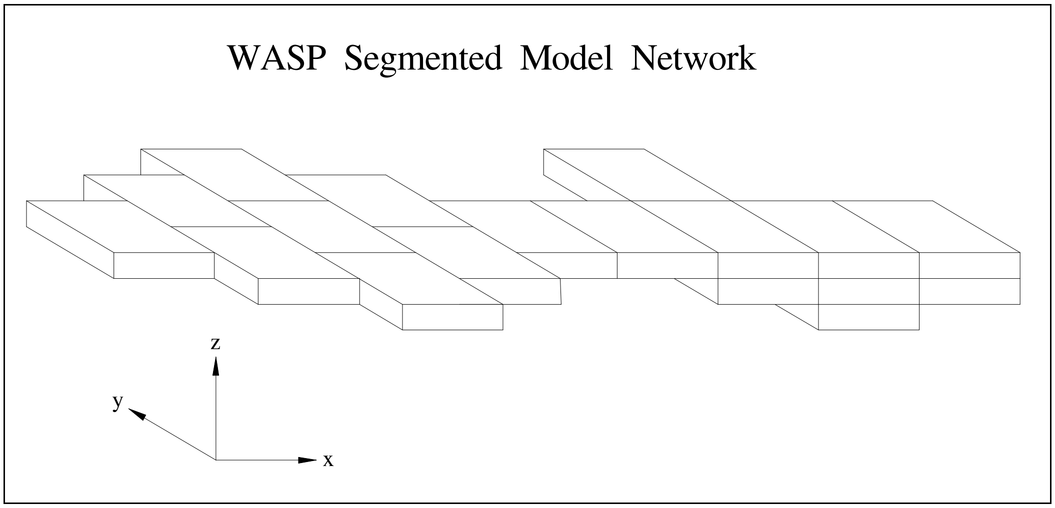

Figure 3.3 WASP6.1 Segmented Model Network
(Adapted from: Wool et al., 2003)

As shown in Figure 3.3, waterbodies can be divided into a series of segments in the longitudinal, lateral, and vertical directions. As a result, WASP6.1 can be used to simulate water quality in 1-, 2-, and 3-dimensions. Therefore, a specific model segment will have adjoining segments either upstream or downstream, on top or on bottom, or from side to side depending on the dimensionality of the water quality simulation. Additionally, if WASP6.1 is linked to DYNHYD5 for hydrodynamics, then WASP model segments will correspond directly to DYNHYD model junctions.

3.2.1 WASP6.1 Model Equations (Wool et al., 2003)

As stated previously, WASP6.1 uses a segmented model network to perform water quality simulations. In order to calculate water quality constituent concentrations, WASP6.1 solves the 3-dimensional mass balance equation within each segment. Wool et al. (2003) presents the mass balance equation (3.15) utilized by the WASP model:

$$\frac{\partial C}{\partial t} = -\frac{\partial (uC)}{\partial x} - \frac{\partial (vC)}{\partial y} - \frac{\partial (wC)}{\partial z} + \frac{\partial}{\partial x}\left(E_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(E_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(E_z \frac{\partial C}{\partial z}\right) + S_L + S_B + S_K \quad 3.15$$

where:
C = water quality constituent concentration (mg/L or g/m^3),
t = time (days),
u = longitudinal advective velocity (m/day),
v = lateral advective velocity (m/day),
w = vertical advective velocity (m/day),
E_x = longitudinal diffusion coefficient (m^2/day),
E_y = lateral diffusion coefficient (m^2/day),

E_z = vertical diffusion coefficient (m^2/day),
S_L = direct/diffuse loading rate (g/m^3-day),
S_B = boundary loading rate (g/m^3-day), and
S_K = kinetic transformation rate (g/m^3-day).

For this research, a 1-dimensional WASP6.1 model was developed for the lower Appomattox River. As a result, equation 3.15 must be modified in order to simulate water quality in the longitudinal direction only. The 1-dimensional advection-diffusion (mass balance) equation is shown in equation 3.16 (Ambrose et al., 2003):

$$\frac{\partial(AC)}{\partial t} = \frac{\partial}{\partial x}\left(-uAC + E_x A \frac{\partial C}{\partial x}\right) + A(S_L + S_B) + AS_K \qquad 3.16$$

Where A is the cross-sectional area (m^2) of the segment, in which the mass balance equation is being solved. The first term of equation 3.16 represents the transport of water quality constituents between adjoining segments. In addition, constituent transport rates are solved along the interfaces of connecting segments. The second term of the equation 3.16 denotes the loading process of water quality constituents. Finally, the third term represents the kinetic transformation process (growth or die-off) of water quality constituents.

WASP6.1 employs a finite difference solution scheme in order to perform calculations. As a result, equation 3.16 must be rewritten in finite difference form, which is shown in equation 3.17:

$$\frac{\Delta(V_j C_j)}{\Delta t} = -\sum_i Q_{ij} C_{ij} + \sum_i R_{ij}(C_i - C_j) + \sum_L V_j S_{Lj} + \sum_B V_j S_{Bj} + \sum_K V_j S_{Kj} \qquad 3.17$$

where:
V_j = volume of segment j (m^3),
C_i = constituent concentration in segment i (mg/L or g/cm^3),
C_j = constituent concentration in segment j (mg/L or g/cm^3),
C_{ij} = interfacial constituent concentration between segments i and j (mg/L or g/cm^3),
t = time (days),
Q_{ij} = interfacial flow between segments i and j (m^3/day), and
R_{ij} = dispersive flow between segments i and j [defined in equation 3.18] (m^3/day).

When using 1-dimensional water quality models of streams, rivers, and estuaries, the mixing effects due to dispersion are typically much greater than the mixing effects due to diffusion (Martin and McCutcheon, 1999). As a result, the diffusion-mixing coefficient (E_x) in the advection-diffusion equation (3.16) is replaced with a dispersion-mixing coefficient that carries the same units (m^2/s). Equation 3.18 (Wool et al., 2003) represents the actual dispersive exchange between two WASP6.1 segments (i and j).

$$\frac{\partial M_{jk}}{\partial t} = \frac{E_{ij} A_{ij}}{L_{ij}}(C_{ik} - C_{jk}) = R_{ij}(C_{ik} - C_{jk}) \qquad 3.18$$

where:
M_{jk} = mass of constituent k in segment j (g),
t = time (days),
E_{ij} = dispersion coefficient for exchange ij (m^2/day),
A_{ij} = interfacial area between segments i and j (m^2),
L_{ij} = characteristic mixing length between segments i and j (m),
C_{ik} = concentration of constituent k in segment i (mg/L or g/m^3), and
C_{jk} = concentration of constituent k in segment j (mg/L or g/m^3).

In addition to advective and dispersive transport, the 1-dimensional, mass balance equation (3.16) is also a function of direct/diffuse loading rates (S_L), boundary loading rates (S_B), and kinetic transformation rates (S_K). Within the WASP6.1 modeling framework, direct/diffuse and boundary loadings rates can be specified directly. However, this is not the case with the kinetic transformation rate. In order to simulate the fate (decay) of fecal coliform bacteria for this research, a first-order transformation rate was utilized. This transformation rate is expressed in equation 3.19:

$$\frac{dC}{dt} = -k\Theta^{(T-20)}C \qquad 3.19$$

where:
C = concentration of coliform bacteria at time t (cfu/100mL),
t = time (days),
k = coliform bacteria die-off rate at 20°C (1/days),
Θ = temperature coefficient (dimensionless), and
T = temperature (°C).

Because the current version of WASP6.1 does not have a fecal coliform function, the research team used the nitrate nitrogen state variable to simulate the fate and transport of fecal coliform bacteria in the lower Appomattox River. The kinetic transformation rate of nitrate nitrogen is expressed in equation 3.20 (Wool et al., 2003):

$$\frac{\partial C_2}{\partial t} = k_{12}\Theta_{12}^{(T-20)}\left(\frac{C_6}{K_{NIT}+C_6}\right)C_1 - G_{P1}\alpha_{NC}(1-P_{NH3})C_4 - k_{2D}\Theta_{2D}^{(T-20)}\left(\frac{K_{NO3}}{K_{NO3}+C_6}\right)C_2 \qquad 3.20$$

where:
C_1 = concentration of ammonia nitrogen at time t,
C_2 = concentration of nitrate nitrogen at time t,
C_4 = concentration of phytoplankton carbon at time t,
C_6 = concentration of dissolved oxygen at time t,
t = time,
k_{12} = nitrification rate at 20°,
k_{2D} = denitrification rate at 20°C,
Θ_{12} = nitrification temperature coefficient,
Θ_{2D} = denitrification temperature coefficient,

T = temperature (°C),
α_{NC} = nitrogen to carbon ratio,
G_{P1} = phytoplankton growth rate,
K_{NIT} = half saturation constant for oxygen limitation of nitrification,
K_{NO3} = Michaelis constant for denitrification, and
P_{NH3} = preference for ammonia uptake.

After setting all of the secondary terms to zero within WASP6.1, equation 3.20 simplifies to equation 3.21:

$$\frac{\partial C_2}{\partial t} = -k_{2D}\Theta_{2D}^{(T-20)}C_2 \qquad 3.21$$

Which is equivalent to the first-order transformation rate for fecal coliform bacteria presented in equation 3.19.

WASP6.1 utilizes a one-step Euler finite difference technique to solve the mass balance equation (3.17) in conjunction with the transformation rate equation (3.21) and the flow data stored within the hydrodynamic linkage file (Wool et al., 2003). The solution method is explicit by nature, and the discrete differences for the dependent variables are expressed in terms of the known time level (t-1), which is shown in equations 3.17. The one-step Euler technique utilizes known values at the beginning of the time interval (t-1) to perform computations across the entire interval (Δt). This process results in a series of values obtained at the end of the time interval (t), which will be used as the starting conditions for the next time step (Boyce and DiPima, 1997). Explicit finite difference techniques are developed in further detail in section 2.4.1.1 of chapter 2.

3.2.2 WASP6.1 Required Inputs (Wool et al., 2003)

Previous versions of the WASP modeling software (WASP4 and WASP5) utilized space-delimited input data files coded in ASCII text. This was a direct result of the model being written in FORTRAN 77 code and implemented through DOS on IBM compatible personal computers. However, the current version of the modeling software (WASP6.1) has been fully integrated into a Microsoft WINDOWS environment. The model code has been converted into a series of dynamic link libraries (DLLs), and an updated WINDOWS-based preprocessor has replaced the old DOS-based program. The new preprocessor completely eliminates the need for text editors and spreadsheets to generate as well as edit WASP input files. In addition, the new WINDOWS-based preprocessor proved to be faster and more efficient than the older DOS-based program. As a result, input file generation and manipulation was greatly simplified.

WASP6.1 input files (WIF extension) are generated with the aid of 13 separate preprocessor screens or options. The 13 options include, but are not limited to data set, systems, segments, parameters, constants, loads, boundaries, and time step. The preprocessor options and their respective inputs are listed and discussed below. Since the WASP6.1 input files used for this research are coded in a WINDOWS-based format, they cannot be printed out and supplied with this report. Therefore, input data files can be obtained from the author of this document (Andrew Hammond, anhammo2@vt.edu). Readers are encouraged to review chapter 3 of the WAPS6 user's manual (Wool et al., 2003) for a complete description of the input data file organization.

<u>Option 1: Data Set</u>

The data set option of the preprocessor enables the user to specify which WASP sub-model will be used for simulations (EUTRO, TOXI, HEAT, Mercury, or Advanced Eutrophication Model). In addition, the user has the ability to provide a simulation description and comments. Within the data set option the user is also prompted to specify the simulation starting date and time as well as hydrodynamic and non-point source file linkages if utilized. Restart and time step options are also provided in the data set option of the preprocessor.

<u>Option 2: Systems</u>

The systems option of the preprocessor enables the user to specify which WASP6.1 state variables will be simulated within the given sub-model. For example, if the user selects the EUTRO sub-model under the data set option, then they have the opportunity to simulate, hold constant, or bypass the 9 EUTRO state variables (ammonia, nitrate, dissolved oxygen, etc.) within the systems option. In addition, the systems option allows the user to specify whether advection, dispersion, or both processes will transport a specific state variable. Also, the user has the capability of specifying state variable density, maximum calculated concentration (used for stability purposes), and boundary in addition to loading scale and conversion factors.

<u>Option 3: Segments</u>

Within the segments option, a model user has the ability to define the number of waterbody segments to simulate as well as their volumes (m^3). In addition, the user can define segment velocity multipliers and exponents, which are used to define segment velocities (m/s) using a power function (3.22):

$$V = aQ^b \qquad 3.22$$

where:
V = segment velocity (m/s),
a = velocity multiplier,
b = velocity exponent, and
Q = segment flowrate (m^3/s).

The same power function approach is used to define segment depths (m) within the WASP6.1 modeling framework. As a result, the user has the ability to define segment depth multipliers and exponents. However, if WASP6.1 is linked to a DYNHYD5 hydrodynamic linkage file, then segment depths and velocities are provided by the linkage file at each computational time step.

Also, within the segments option initial concentrations for each state variable are specified for each segment. In addition, the dissolved fraction of each state variable is defined for each segment. Finally, the user must specify segment parameter values such as temperature (°C), light extinction, sediment oxygen demand, incoming solar radiation, etc.

<u>Option 4: Parameters</u>

The parameters option allows the model user to determine which segment parameters will be used during a given simulation. In other words, segment parameters can be turned off and on during different simulations simply by checking a box. This allows the model user to quickly determine the influence of a given parameter on model results just by turning it off or on. In addition, the user can specify a parameter scale factor, which can be used to increase or decrease the value of a given parameter.

<u>Option 5: Constants</u>

The constants option allows the user to specify model constants for each state variable being simulated. For example, the nitrate nitrogen constants include the denitrification rate at 20°C, denitrification temperature coefficient, and half saturation denitrification oxygen limit. Therefore, within the nitrate nitrogen constant group model users can specify a value for each of the constants as well as tell the model if they will be used for a given simulation similar to the process used for model parameters.

<u>Option 6: Exchanges</u>

The exchanges option enables model users to define dispersion transport for surface water exchanges as well as pore water exchanges. For each exchange field (surface water or pore water), the user can establish 10 different exchange functions if necessary. Within an exchange function, WASP6.1 segments are paired together denoting their linkage, and their interfacial mixing area (m^2) and characteristic mixing length (m) are specified. In addition, a dispersion coefficient (m^2/s) for the given exchange is defined for the function. The use of 10 different exchange functions allows the user to vary the dispersion coefficient between segment pairs if required.

<u>Option 7: Flows</u>

The flow option of WASP6.1 works in the same manner as the exchanges option. Model users can define flowrates (m^3/s) for surface water, pore water, evaporation/precipitation, and solids. For each flow field, users can define 10 different flow functions if needed. Within each flow function, segments are paired together defining how the flow moves from segment to segment. In addition, the user must specify the fraction of the total flow that moves from segment to segment within a pair. Finally, the flowrate is established for a given flow function, therefore, defining the flowrate for segments pairs within that function. If a DYNHYD5 hydrodynamic linkage file is used, then model users will not have the capability to specify additional flows within the WASP6.1 model. Flowrates will be read in from the DYNHYD5 hydrodynamic linkage file at each computational time step.

Option 8: Loads

The WASP6.1 loads option provides the user the opportunity to specify waste loads (direct/diffuse loading rates) for simulated state variables within a given segment. For each segment containing waste loads, the user must specify the state variable's time-variable loading rate (kg/day). The loading rate is defined using date, time, and value (kg/day) parameters, and the maximum number of break points (4000) was not exceeded for this research. Also, the user has the ability to specify loading rate scale and conversion factors if necessary.

Option 9: Boundaries

WASP6.1 requires the user to specify boundary conditions for each state variable being simulated. This is accomplished by specifying time-variable boundary concentrations (mg/L) for each state variable at every model boundary. The parameters associated with time-variable boundary conditions are date, time, and concentration. In addition, the boundary option provides the user the opportunity to specify concentration scale and conversion factors if required.

Option 10: Time Functions

The WASP6.1 time functions option allows the model user to specify time-variable functions for a number of different model parameters including: water temperature, solar radiation, wind speed, light extinction, water velocity, ammonia benthic flux, phosphorus benthic flux, air temperature, and ice cover. These time functions enable the user to vary specific model parameters in order to access their impacts on model simulation results. Parameters for each time function include date, time, and value (with respective units).

Option 11: Print Interval:

The print interval option enables the user to tell the model at what specific time interval to print results to the output file. The model print interval does not have to remain constant and can be changed with the use of a time-variable print interval. This enables model users to view output at shorter or longer intervals if necessary. Inputs associated with the print interval are date, time, and print interval (days).

Option 12: Time Step

The model time step is specified using the time step option within the WASP6.1 preprocessor. As is the case with the mode print interval, the model time step does not have to remain constant and can be changed with the aid of a time-variable time step. This enables the user to perform calculations at longer or shorter time steps during a single simulation if required for model stability. Inputs associated with the model time step are date, time, and time step (days). If a DYNHYD5 hydrodynamic linkage file is employed, then the WASP6.1 model time step is predefined within the linkage file and does not have to be established. See Group C: Hydraulic Summary for more information concerning the WASP6.1 time step and the DYNHYD5 hydrodynamic linkage file.

Option 13: Validate Input

The validate input option verifies that the input data provided by the model user is within the given capabilities of the selected WASP6.1 sub-model (Wool et al., 2003). It will notify model users if required model inputs are missing or undefined. However, the validate input option will not check to see if model inputs are well outside of expected ranges. The validity of model inputs is the responsibility and burden of the user.

3.2.3 WASP6.1 Model Stability

Computation stability and numerical accuracy of the WASP6.1 model is a function of segment volumes and simulation time step. As segment volumes increase or decrease (typically due to flood and ebb tides), the model time step must also increase or decrease to assure model accuracy and stability (Wool et al., 2003). As a result, WASP6.1 has the ability to automatic time step (modify model time step with respect to segment volumes) in order to insure stability throughout a simulation run. However, this is not the case when linking WASP6.1 to DYNHYD5 with the aid of a hydrodynamic linkage file.

When using a DYNHYD5 hydrodynamic linkage file within WASP6.1, the water quality simulation time step is fixed by the ratio of hydrodynamic time steps to water quality time steps. This parameter is specified in DYNHYD5's data group C (Hydraulic Summary) and is transferred over to WASP6.1 within the hydrodynamic linkage file. Therefore, to insure stability and numerical accuracy of WASP6.1, users must specify a reasonable water quality time step within DYNHYD5. Next, they should perform a series of water quality simulations to assure that the selected time step has no ill effects on WASP6.1 simulation calculations and results. WASP6.1 instabilities are typically an indication that the simulation time step must be reduced within DYNHYD5 and subsequently within the hydrodynamic linkage file.

4.0 Model Application to Lower Appomattox River, Virginia

Chapter 4 details input file generation for hydrodynamic and fecal coliform simulation within the lower Appomattox River using the DYNHYD5 and WASP6.1 modeling software. Time period selection for model sensitivity analysis, calibration, and validation is also discussed briefly.

4.1 Model Study Area: Lower Appomattox River, Virginia

The Appomattox River is part of the James River basin, located in central Virginia, with an outlet approximately 25 miles southeast of Richmond, Virginia. This is reflected in Figure 4.1 below. The Appomattox River flows in an easterly direction before emptying into Lake Chesdin, a reservoir on the Appomattox River. The Appomattox River continues to flow in an easterly direction and joins Swift Creek, ultimately emptying into the James River at Hopewell, Virginia. The Appomattox River watershed is located within the Appomattox River hydrologic unit, United States Geological Survey (USGS) number 02080207. The drainage area of the Appomattox River watershed is approximately 4146 km^2 (1600 mi^2) with 71% forested, 19% agricultural, 7% water and/or wetlands, 2% residential, and 1% commercial.

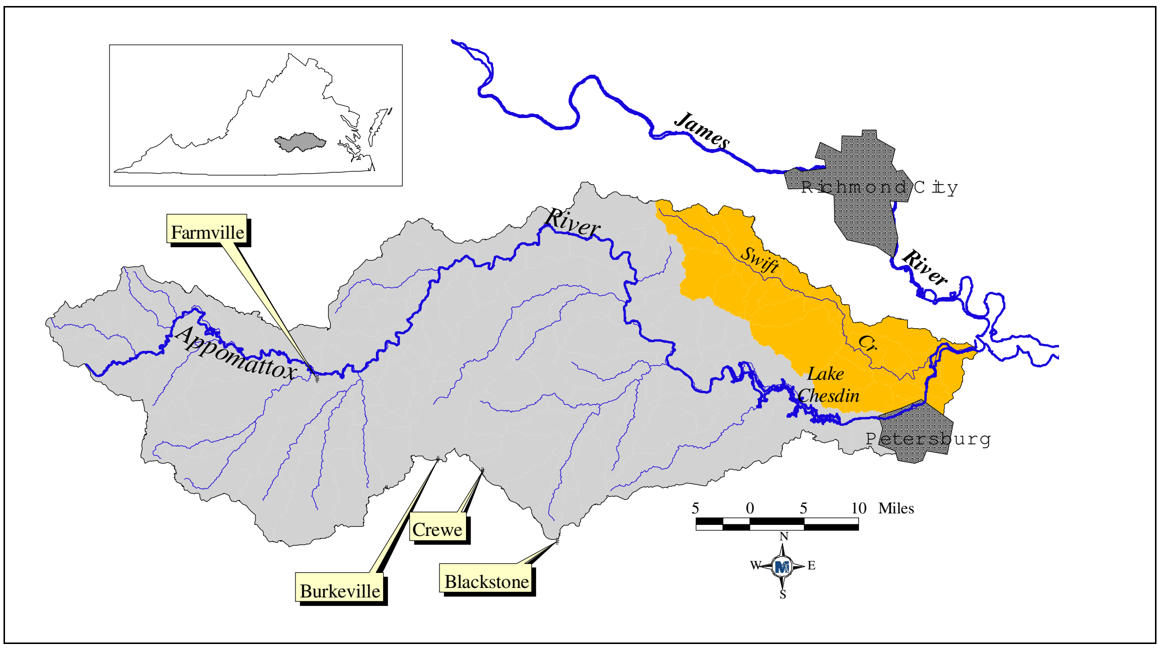

Figure 4.1 Model Study Area: Appomattox River, VA

The tidal Appomattox River is part of the lower Appomattox River watershed with an outlet in Hopewell, Virginia. The tidal portion of the Appomattox River begins in Petersburg, Virginia and flows in an easterly direction. Swift Creek joins the Appomattox River after passing through the Swift Creek Reservoir. The Appomattox River continues to flow in an easterly direction, eventually emptying into the James River. The immediate drainage area of the tidal Appomattox River is highlighted in orange in Figure 4.1. The area of the tidal Appomattox River is approximately 624 km^2

(241 mi^2) or 15% of the total watershed. The tidal land area is 72% forested, 12% agricultural, 7% residential, 6% water and/or wetlands, and 2% commercial (Petrauskas, 4/21/03).

Portions of the Appomattox River have been listed as impaired by USEPA due to high bacteria (fecal coliform) concentrations. One impaired segment of interest is the tidal portion of the Appomattox River. This river segment is approximately 16.9 km (10.5 mi) long and passes through the cities of Colonial Heights, Petersburg, and Hopewell (VADEQ, 2002). Due to the tidal influence, the Appomattox River is an ideal study area for research on model implementation and the prediction of hydrodynamics and water quality in tidally influenced areas.

4.2 Data Collection and Processing

The assembly of DYNHYD5 and WASP6.1 input data files for the lower Appomattox River presents a considerable challenge. MapTech, Inc. of Blacksburg, Virginia provided the existing HSPF and Geographic Information System (GIS) data sets used during the input file generation process. These data sets will be discussed in later sections detailing DYNHYD5 and WASP6.1 input file generation. However, a significant amount of new data was collected and processed in order to complete the generation of the necessary input files. These data sets are discussed briefly in the following sections.

4.2.1 NOAA Tide Predictions

DYNHYD5 requires model users to provide boundary conditions for all upstream and downstream boundaries contained within the model network. Boundary conditions include model inflows for upstream boundaries, model outflows for downstream boundaries or time-variable tidal heights for downstream boundaries. The downstream DYNHYD5 boundary for this research was established and the most appropriate boundary condition was chosen.

The Appomattox River flows in an easterly direction until it empties into the James River at City Point in Hopewell, Virginia. The confluence of the Appomattox River with the James River serves as the downstream DYNHYD5 boundary for this research. In addition, the Appomattox River and the James River are both tidally influenced. As a result of the tidal influence, the USGS does not operate or maintain a streamflow gage near or around Hopewell, Virginia. This is due to the fact that streamflow measurements are determined with the aid of rating curves, which are linked directly to river stage (depth). However, in tidally influenced waters, a given river stage can have a number of different streamflows associated with it, which is directly related to the coupling of dry or wet weather flows with flood or ebb tides. Due to the highly complicated relationship between tidal height and streamflow as well as the lack of a USGS streamflow gage, model outflows were not chosen as the downstream boundary condition for this research.

In addition to the lack of a USGS streamflow gage, the National Oceanic and Atmospheric Administration (NOAA) does not currently operate a tidal stage recorder at the confluence of the Appomattox and James Rivers. Therefore, real-time tidal heights could not be utilized as the downstream boundary condition within DYNHYD5. However, near the end of each calendar year (approximately November), NOAA releases (to the public) tide predictions for a number of different locations throughout the United States for the following calendar year. City Point in Hopewell, Virginia is one location in which NOAA predicts and releases. As a result, NOAA tide predictions were used as the input for the downstream DYNHYD5 model boundary.

Sixteen years of tide predictions (1988 through 2003) were obtained from NOAA on a single 3.5" floppy diskette. The tide predictions were provided in NOAA standard format utilizing military time with daylight savings time taken into consideration. A sample of the tide predictions obtained from NOAA is provided in Appendix E. It should be noted that NOAA tide predictions include the high and low predicted tidal heights (meters, referenced from mean lower low water) with their predicted time of occurrence for a given day. Therefore, for the Appomattox River, this equates to 3 or 4 data points (predictions) each day.

Microsoft Excel was utilized to reformat the tide predictions from NOAA standard format to DYNHYD5 input format. Sample tide predictions in DYNHYD5 format are provided below in Table 4.1. Days 1, 2, and 3 correspond to January 1, 2003, January 2, 2003, and January 3, 2003 respectively.

Table 4.1 Sample Tide Predictions in DYNHYD5 Format.

Day	Hour	Minute	Tidal Height (m)
1	1	43	3.994
1	8	4	3.171
1	13	59	4.146
1	21	4	3.141
2	2	36	3.994
2	8	59	3.171
2	14	52	4.146
2	21	56	3.141
3	3	27	3.994
3	9	53	3.171
3	15	43	4.116
3	22	44	3.141

4.2.2 Continuous, Time-Variable Tidal Heights

To facilitate the calibration and validation of the DYNHYD5 hydrodynamic model, the researchers installed a recording tidal height gage at the Hopewell City Marina. The marina is located slightly upstream from City Point and is not contained within the downstream boundary of the DYNHYD5 model network. The tidal stage recorder (pressure transducer and data collector) was installed at Hopewell City Marina on May 22, 2003 under the permission and supervision of Jo Turek, Director of Parks and Recreation, City of Hopewell, Virginia.

The data collection device was configured to take stage readings every 30 minutes on the hour and half-hour. Tidal heights were downloaded from the data collector approximately every 30 days with the aid of a laptop computer. In addition, the raw data was processed with Microsoft Excel. After processing, collected data points were placed within a Microsoft Access database for use by the DYNHYD5/WASP6.1 postprocessor during DYNHYD5 calibration and validation. Sample unprocessed tidal heights are shown in Appendix F. Sample processed tidal heights are shown below in Table 4.2.

Table 4.2 Sample Processed Tidal Heights

DATE_TIME	STATION_ID	PCODE	RESULT (m)
5/22/03 11:30	2APP001.53	Height	3.93
5/22/03 12:00	2APP001.53	Height	3.86
5/22/03 12:30	2APP001.53	Height	3.80
5/22/03 13:00	2APP001.53	Height	3.74
5/22/03 13:30	2APP001.53	Height	3.68
5/22/03 14:00	2APP001.53	Height	3.62
5/22/03 14:30	2APP001.53	Height	3.57
5/22/03 15:00	2APP001.53	Height	3.52
5/22/03 15:30	2APP001.53	Height	3.47
5/22/03 16:00	2APP001.53	Height	3.42
5/22/03 16:30	2APP001.53	Height	3.40
5/22/03 17:00	2APP001.53	Height	3.41
5/22/03 17:30	2APP001.53	Height	3.48

The tidal stage recorder remained operational from May 22, 2003 to September 13, 2003, with a data gap from July 5, 2003 to August 8, 2003 due to a faulty battery. The pressure transducer and data collector were removed from the marina shortly after Hurricane Isabel. During the time period of operation, 3819 data points were collected on a 30-minute interval and have been incorporated into this research.

4.2.3 Bathymetry Data

To establish junction bottom elevations (measured from a common datum) as well as channel hydraulic radii, the researchers collected bathymetry data along the Appomattox River and the Appomattox Canal. Thirty-three cross-sections (perpendicular to the longitudinal direction of flow) were taken with the aid of a boat and a depth finder. A global positioning system (GPS) unit was utilized to determine the location of the cross-sections within the river system. Figure 4.2 is a plot of cross-section location along the river, which was used to relate the cross-sections to their respective DYNHYD5 channel number.

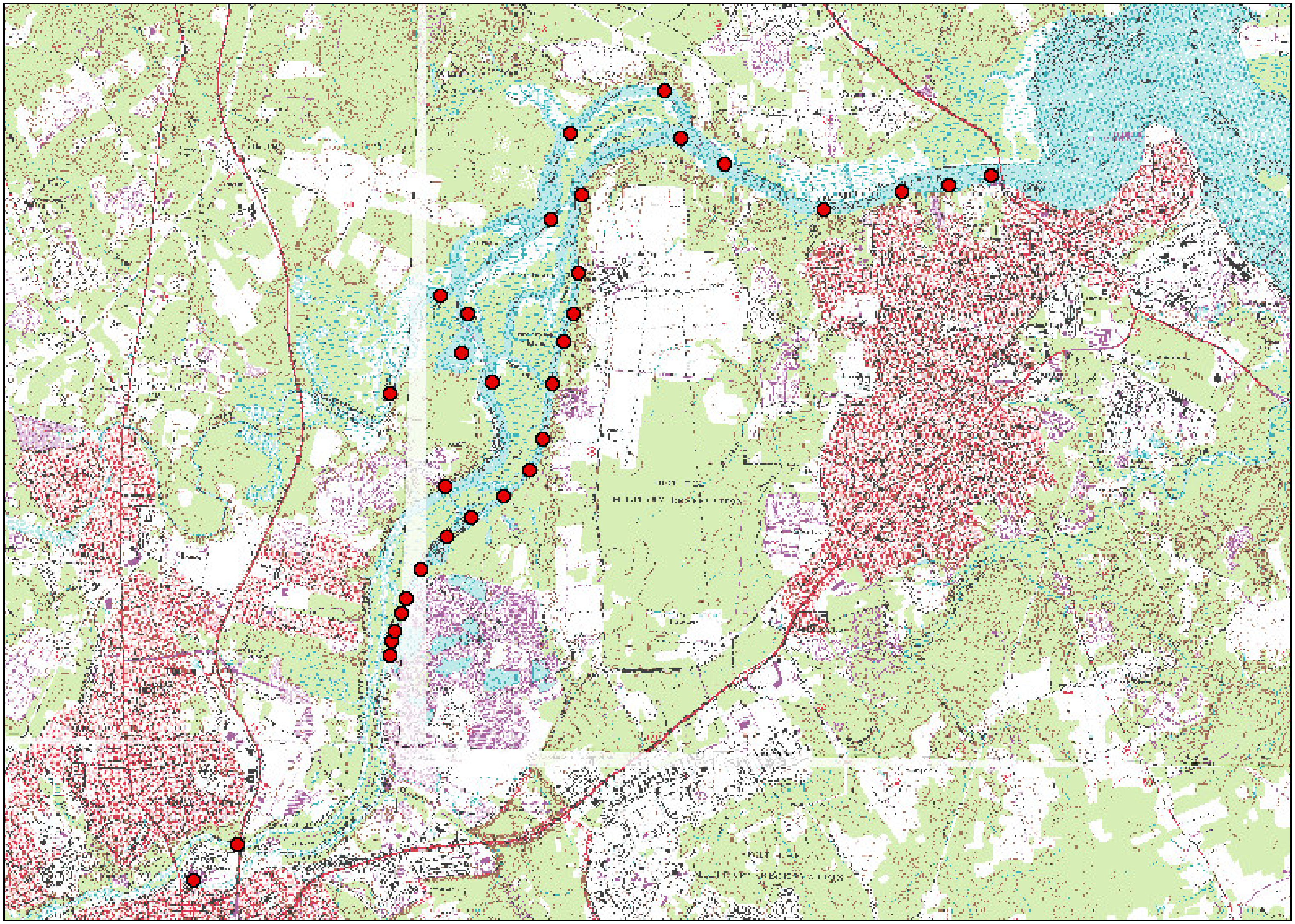

Figure 4.2 ArcView Plot of Cross-section Location

After collecting the necessary cross-sections, the bathymetry data was processed with the aid of Microsoft Excel. DYNHYD5 utilizes the assumption that irregular channel cross-sections can be represented with hydraulically equivalent (hydraulic radius remains approximately the same) rectangular cross-sections. As a result, the bathymetry data was processed to determine the average depth of each cross-section, assuming the top-width of each cross-section remained constant. The calculated average depths are shown below in Table 4.3.

Table 4.3 Cross-section Average Depths

Cross-section	Average Depth (m)
1	4.51
2	2.45
3	4.54
4	6.67
5	3.45
6	2.62
7	4.11
8	3.40
9	1.57
10	1.54
11	1.14
12	0.74
13	1.25
14	1.62
15	1.90
16	2.07
17	2.07
18	2.23
19	2.24
20	2.55
21	2.56
22	2.58
23	2.60
24	2.45
25	2.46
26	2.48
27	2.49
28	2.50
29	2.50
30	3.62
31	1.44
32	1.49
33	1.07

Cross-section average depths were then used to verify and refine the bathymetry data contained on the 4 USGS 7.5-minute quadrangle sheets covering the tidal Appomattox River.

4.3 DYNHYD5 Input File Generation

A significant amount of data was collected and processed to generate DYNHYD5 input files for model calibration, validation, and sensitivity analysis. Model junction data, channel data, and DYNHYD5 to WASP6.1 map data remained constant and did not vary between calibration, validation, and sensitivity analysis simulation runs. For brevity, the generation of the DYNHYD5 input file used for model calibration and sensitivity analysis is discussed below. The calibrated DYNHYD5 input file is shown in Appendix D. The generation process remains the same for the input files created for model validation.

The DOS-based DYNHYD5 preprocessor (PREDYN) was used initially to generate the required calibration and sensitivity analysis input file. PREDYN provides users with a series of input screens in which they provide specific model inputs. At the completion of data entry, PREDYN saves the data, in ASCII format, in a DYNHYD5 input file (INP file extension). Since the input file is coded in ASCII format, a text editor may be used to perform changes. As a result, TextPad4.7.1 was used for the remainder of this research to generate and edit DYNHYD5 input files. The use of a text editor proved to be fast and efficient when manipulating input files for different simulation runs.

For model calibration, validation, and sensitivity analysis wind effects were not taken into account. This is due to the fact that local wind data (speed and direction) was not available at the time of input file generation. In addition, due to a lack of detailed bathymetry data, the variable junction and channel geometry options within DYNHYD5 were not utilized. Therefore, junction surface areas and channel top-widths do not vary with water surface elevation. As a result, the model perceives channels and junctions as rectangular in cross-section.

4.3.1 Model Segmentation

MapTech, Inc. of Blacksburg, Virginia provided assistance for the ArcView GIS software as well as the existing GIS datasets used in DYNHYD5 segmentation. Portions of the National Hydrodraphy Dataset (NHD) containing the tidal Appomattox River were plotted using ArcView. In addition, pre-established HSPF subsheds were plotted on the same drawing. Twenty-three junction locations were chosen along the Appomattox River and Appomattox Canal. Where possible, model junctions were placed at the same location of HSPF subshed outlets. In addition, junction spacing (channel length) was held relatively constant throughout the model network to insure model stability. The placement of model junctions automatically led to the definition of 29 model channels. Figure 4.3 is an ArcView location plot of the junction (labeled in the figure) and channel network used in model calibration and sensitivity analysis.

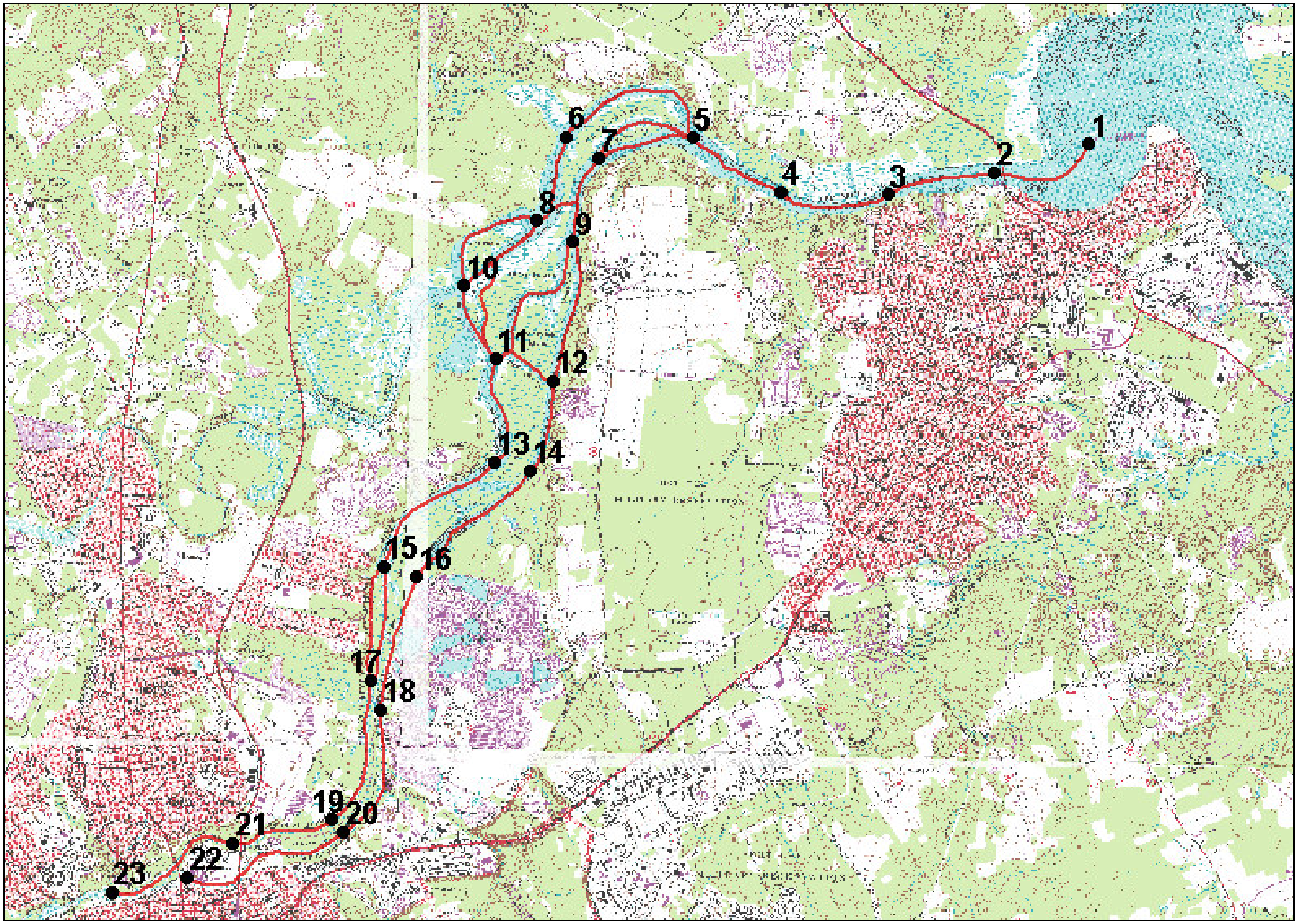

Figure 4.3 ArcView Plot of Link-Node Model Network

The modified version of DYNHYD5 (provided by USEPA) used for this research employs a junction and channel numbering convention, which starts upstream (junction/channel number 1) and works downstream (junction/channel number N) in the "positive" direction of flow. However, this was unknown at model setup. As a result, the numbering convention presented in the DYNHYD5 user's manual (Ambrose et al., 1993a) was utilized, which starts downstream and works upstream. The DYNHYD5 positive direction of flow for the Appomattox River is now considered to be downstream to upstream. Consequently, flowrates and velocities for water leaving the system to the James River are now represented as negative numbers in the DYNHYD5 output file, which is opposite from typical convention.

4.3.2 Channel Data (Data Group E)

ArcView in conjunction with the NHD was used to determine the average top-width of each model channel. To do so, approximately 5 measurements of top-width were taken along the length of each channel. These measurements were then averaged to determine an average top-width for each channel. In addition to channel widths, channel lengths were established with the aid of ArcView. Within DYNHYD5, channel length is defined as the distance from junction center to junction center. As a result, these distances were easily measured with the ArcView software.

NOAA bathymetry data contained on 4 USGS 7.5-minute quadrangle sheets (Hopewell, VA; Prince George, VA; Chester, VA; Petersburg, VA) was used to determine the hydraulic radius (average channel depth) for each channel. As previously stated, DYNHYD5 utilizes the assumption that irregular channel cross-sections can be represented with hydraulically equivalent (hydraulic radius remains approximately the same) rectangular cross-sections. The hydraulic radius of a rectangular channel is given by equation 4.1:

$$R = \frac{BD}{B + 2D} \qquad 4.1$$

where:
R = hydraulic radius (m),
B = channel width (m), and
D = channel depth (m).

It is well known that for a rectangular channel whose width is 10 times greater that its depth, the hydraulic radius is approximately equal to its depth. This assumption is commonly referred to as the wide channel approximation. Therefore, the width to depth ratio was determined for each DYNHYD5 channel, and all calculated ratios were greater than 10. As a result, channel hydraulic radius was replaced with average channel depth within the DYNHYD5 input file. Therefore, average channel depths were determined with the aid of NOAA bathymetry data contained on the 4 previously mentioned USGS quadrangle sheets. These depths were revised and refined with the help of the previously obtained cross-section average depths.

To determine channel directions, Figure 4.3 was exported from ArcView in AutoCAD format. AutoCAD was then employed to measure the direction of each channel in degrees from true north. Within DYNHYD5, channel direction is defined as pointing in the direction of positive flow. Therefore, channel directions were measured from lower junction number to higher junction number (downstream to upstream), which is the direction of positive flow for this research.

While collecting bathymetry data on the Appomattox River, the research team paid close attention to river bed and bank vegetation. This was done in order to establish a Manning's roughness coefficient (n-value) for each channel in the model network. Figures from Chow (1959) were used to provide initial estimates of Manning's n-values for each channel. In addition, Manning's roughness coefficients served as the main DYNHYD5 parameter used for model calibration.

Due to a lack of velocity measurements, the initial velocity of each channel was assumed to be 0.00 m/s. DYNHYD5 convergence to an accurate solution was rather quick and occurred at the beginning of the provided model warm-up period (January 1, 2003 through May 21, 2003). In addition to initial velocities, upstream and downstream connecting junctions for each channel were specified with the aid of Figure 4.3. A summary of the channel data used for DYNHYD5 calibration and sensitivity analysis is shown below in Table 4.4.

Table 4.4 Summary of DYNHYD 5 Channel Data

Channel Number	Length (m)	Width (m)	Depth (m)	Direction (degrees)	Manning's n-value	Initial Velocity (m/s)
1	1298.05	707.79	3.76	254.00	0.035	0.00
2	1282.16	220.40	3.76	262.00	0.035	0.00
3	1316.99	157.87	3.46	267.00	0.035	0.00
4	1256.71	204.14	3.31	301.00	0.035	0.00
5	1151.01	191.99	2.39	250.00	0.035	0.00
6	1328.92	157.75	2.39	250.00	0.035	0.00
7	2060.23	156.35	3.10	252.00	0.035	0.00
8	1071.10	179.22	1.63	187.00	0.035	0.00
9	1120.92	3.92	2.33	266.00	0.035	0.00
10	1095.27	270.31	3.04	189.00	0.035	0.00
11	1697.51	148.70	1.63	189.00	0.035	0.00
12	1885.10	156.30	1.63	212.00	0.035	0.00
13	1963.02	11.58	2.33	181.00	0.035	0.00
14	1159.30	152.28	2.23	230.00	0.035	0.00
15	1461.19	144.21	2.23	231.00	0.035	0.00
16	853.03	29.23	1.83	128.00	0.035	0.00
17	959.43	127.75	1.73	153.00	0.035	0.00
18	1095.75	104.23	1.83	190.00	0.035	0.00
19	1341.62	155.73	1.98	178.00	0.035	0.00
20	1885.07	114.55	1.37	228.00	0.035	0.00
21	1866.53	155.80	1.45	226.00	0.035	0.00
22	1617.05	58.68	0.91	193.00	0.035	0.00
23	1390.19	67.52	1.14	185.00	0.035	0.00
24	1408.52	45.96	1.14	183.00	0.035	0.00
25	1622.74	64.23	0.91	185.00	0.035	0.00
26	1774.48	57.09	1.22	187.00	0.035	0.00
27	2046.78	72.39	0.91	252.00	0.035	0.00
28	1243.81	49.52	0.91	257.00	0.035	0.00
29	1760.46	55.48	0.91	245.00	0.035	0.00

4.3.3 Junction Data (Data Group D)

DYNHYD5 requires an initial head or water surface elevation (referenced from a common horizontal model datum) to be specified for each junction at model start. For simplicity, all junction initial heads were set equal to initial head of the most downstream junction (1), which is 3.73 m. This initial head corresponds to the first water surface elevation (NOAA tide prediction) specified for the downstream seaward boundary (junction 1) at model start. DYNHYD5 convergence to an accurate solution was rather quick and occurred at the beginning of the provided model warm-up period (January 1, 2003 through May 21, 2003). As a result, the junction initial heads did not have to be modified to successfully execute DYNHYD5.

Within the DYNHYD5 model architecture, junction surface area is defined as the sum of one-half the surface area of all channels entering or exiting the junction. After determining channel widths and lengths with ArcView, a Microsoft Excel spreadsheet was used to calculate the respective surface area for each model junction.

In addition to surface area, DYNHYD5 requires users to specify bottom elevations (referenced from a common horizontal model datum) for each junction. The model datum chosen for this research is the river bottom at the downstream seaward boundary (junction 1). For simplicity, a datum elevation of 0.00 m was chosen for the riverbed. NOAA bathymetry data provided on the 4 previously mentioned USGS 7.5-minute quadrangle sheets was used to establish junction bottom elevations above the horizontal model datum.

DYNHYD5 allows model users to specify a maximum of 6 channels entering or exiting a single junction in order to simulate complex branching river networks. As a result, channel numbers corresponding to those entering or exiting each junction were determined with Figure 4.3 and specified within the input data file. A summary of the junction data used for DYNHYD5 calibration and sensitivity analysis is presented in Table 4.5 below.

Table 4.5 Summary of DYNHYD5 Junction Data

Junction Number	Initial Head (m)	Surface Area (m^2)	Bottom Elev. (m)
1	3.73	459373.40	0.00
2	3.73	600667.44	0.00
3	3.73	245250.64	1.02
4	3.73	232229.00	0.61
5	3.73	504640.64	1.32
6	3.73	309089.70	1.02
7	3.73	313488.04	2.44
8	3.73	355222.31	1.45
9	3.73	369511.70	2.85
10	3.73	254911.80	2.64
11	3.73	336902.32	2.44
12	3.73	195781.91	2.44
13	3.73	249867.93	2.14
14	3.73	165072.40	2.44
15	3.73	224703.29	2.75
16	3.73	155411.63	3.36
17	3.73	129953.14	2.75
18	3.73	99558.54	3.36
19	3.73	81449.27	3.36
20	3.73	126197.50	3.36
21	3.73	79631.90	3.36
22	3.73	74083.20	3.36
23	3.73	48835.16	3.36

4.3.4 Inflow Data (Data Group F)

MapTech, Inc. of Blacksburg, Virginia, developed a calibrated and validated HSPF model for the entire Appomattox River basin. Time-variable, daily-averaged, HSPF streamflows (m^3/s) were used as inputs to the DYNHYD5 model network. More specifically, junctions 6 (Ashton Creek), 10 (Swift Creek), 17 (Oldtown Creek), and 23 (Appomattox River – Main Stem) received 212 (January 1, 2003 through July 31, 2003) time-variable, daily-averaged, HSPF streamflows, which also take into account overland inflow. These streamflow locations represent the 4 major flow inputs to the tidal Appomattox River. Due to the vast amount of data (848 data points total), the 4 major junction inflows will not be presented here. However, they are shown in their entirety in the sample DYNHYD5 input file presented in Appendix D.

Time-variable, daily-averaged, HSPF overland flows (m^3/s) were utilized as flow inputs for the remaining 19 model junctions. A sensitivity analysis was performed on the overflow flow inputs (presented in chapter 4), and it was determined that they have an insignificant impact on model results. Therefore, the 212 time-variable, daily-averaged overland flows for each of the remaining 19 junctions were averaged to create a single constant overland flow for each junction. The constant overland inflows with respective junction number are shown below in Table 4.6.

Table 4.6 Constant DYNHYD5 Overland Inflows

Junction Number	Inflow (m^3/s)
1	0.011
2	0.072
3	0.399
4	0.072
5	0.060
7	0.016
8	0.043
9	0.034
11	0.028
12	0.020
13	0.048
14	0.122
15	0.043
16	0.071
18	0.194
19	0.023
20	0.497
21	0.039
22	0.138

It should be noted that within the DYNHYD5 model architecture, inflows are represented as negative numbers and outflows are represented as positive numbers. This should be taken into consideration when creating DYNHYD5 input files that contain either constant or time-variable inflows or outflows.

4.3.5 Seaward Boundary Data (Data Group G)

For this research, junction 1 (confluence of Appomattox River and James Rivers) was designated as the downstream model boundary or seaward boundary. Therefore, a series of boundary conditions are required at DYNHYD5 junction 1. For this research, high and low tidal heights versus time were specified for entire simulation period (212 days). As noted in section 4.2.1, NOAA does not operate or maintain a tidal stage recorder near or around City Point (confluence of Appomattox and James Rivers) in Hopewell, Virginia. As a result, the NOAA tide predictions (high and low tidal heights versus time) for City Point were used as the boundary conditions for the downstream seaward boundary. A further discussion of the NOAA tide predictions as well as their processing required for use is presented in section 4.2.1 of this chapter.

4.3.6 Simulation Control, Printout Control, and Hydraulic Summary (Data Groups A, B, and C)

The number of junctions (23) and channels (29) within the DYNHYD5 model network was established during segmentation, and they are shown in Figure 3.6. The shortest channel length was determined to be 853.03 m, which corresponds to channel 16. The average depth of channel 16 is 1.83 m, and the average velocity was determined to be approximately 0.19 m/s. The model time step calculated with the Courant-Friedrichs-Lewy stability criteria (presented in equation 3.14) was 192 sec. This was rounded down to 180 sec (3 min) for simplicity. However, initial DYNHYD5 simulation runs proved to be unstable at a model time step of 180 sec. Therefore, the time step was reduced to 30 sec, at which point satisfactory model results were obtained.

DYNHYD5 calibration and sensitivity analysis runs began on day 1 (January 1, 2003 12:00 AM) and ended on day 212 (July 31, 2003 12:00 AM). Printout of model simulation results for all 23 junctions and 29 channels began at model time zero (January 1, 2003 12:00 AM), and results were printed out every half-hour. As a result, a significant amount of data was collected and printed within each output file (BMD extension). In addition, DYNHYD5 output file sizes were approximately 20 MB in size.

DYNHYD5 external hydrodynamic linkage files were created for use with WASP during WASP6.1 calibration, validation, and sensitivity analysis. The creation of hydrodynamic linkage files for WASP utilization began at DYNHYD5 model time zero for all 3 instances. In addition, the ratio of hydrodynamic time steps per water quality time step was set at 30. Therefore, the time step of the WASP6.1 water quality model was fixed at 900 sec or 15 min, which proved to be quite stable during water quality simulations.

4.3.7 DYNHYD Junction to WASP Segment Map (Data Group L)

Creation of an external hydrodynamic linkage file for use with WASP6.1 requires that DYNHYD5 junctions be mapped on to their respective WASP6.1 segments. It should be noted that hydrodynamic model boundaries are assigned a WASP6.1 segment identification of '0'. This boundary labeling convention is utilized in order to tell the water quality model that a model boundary exists when importing the hydrodynamic linkage file. The DYNHYD5 junction to WASP6.1 segment map used for this research is shown below in Table 4.7.

Table 4.7 DYNHYD5 Junction to WASP6.1 Segment Map

DYNHYD Junction	WASP Segment
1	0
2	1
3	2
4	3
5	4
6	5
7	6
8	7
9	8
10	9
11	10
12	11
13	12
14	13
15	14
16	15
17	16
18	17
19	18
20	19
21	20
22	21
23	0

All parameters discussed in the generation of the DYNHYD5 input file used for model calibration and sensitivity analysis can be seen in their entirety in the sample file provided in Appendix D. Readers are urged to review chapters 1 and 2 of the DYNHYD5 user's manual (Ambrose et al., 1993a) for a more thorough discussion of model parameters.

4.4 WASP6.1 Input File Generation

A significant amount of data was collected and processed to generate WASP6.1 input files for model calibration, validation, and sensitivity analysis. For brevity, the generation of the WASP6.1 input file used for model sensitivity analysis is discussed here. WASP6.1 input files are not coded in ASCII format and cannot be printed out in their entirety. Therefore, WASP6.1 input data files can be obtained from the author of this document (Andrew Hammond, anhammo2@vt.edu). The process utilized for input file generation remains the same for the input files created for model calibration and validation.

The WINDOWS-based preprocessor, provided with the WASP6.1 modeling software, was utilized to generate the required input file. The preprocessor provides the user with a series of input screens in which data is entered. At the completion of data entry, the preprocessor saves the data in a WASP6.1 input file (WIF file extension). Unlike previous versions of the WASP modeling software, WASP6.1 does not use an input file coded in ASCII format. As a result, text editors or spreadsheets cannot be used to modify input files. Therefore, the WASP6.1 preprocessor was used throughout this research for water quality input file generation.

4.4.1 Sub-Model Selection and Initial Setup

Due to lack of a specific function for fecal coliforms, the research team used the nitrate nitrogen state variable to simulate the fate and transport of fecal coliform bacteria (see section 3.2.1 of chapter 3 for a more through discussion on the use of the nitrate nitrogen state variable). The EUTRO (eutrophication) sub-model within WASP6.1 was chosen since it contains the nitrate nitrogen state variable and the respective transformation kinetics are discussed in section 3.2.1 of chapter 3.

For WASP6.1 sensitivity analysis, the model start date and start time were set to January 1, 2003 at 12:00 AM. The hydrodynamic linkage option was chosen, and the location of the DYNHYD5 hydrodynamic linkage file was specified. In addition, the no restart file option was selected, and the model time step was set to user defined.

For more information concerning sub-model selection and initial setup, readers are encouraged to read the Input Parameterization section of the WASP6.1 user's manual (Wool et al., 2003).

4.4.2 Model Systems

Within the preprocessor systems screen, the coliforms (nitrate nitrogen) state variable was simulated. The maximum concentration was specified as 9,999,999 cfu/100mL, therefore, effectively telling the model to cease simulation if the maximum concentration is encountered. HSPF water quality simulation runs utilized a fecal coliform bacteria density of 1.00 g/cm^3. Therefore, the default coliforms (nitrate nitrogen) density remained unchanged. In addition, the boundary/loading scale and conversion factors remained unchanged at 1.00.

4.4.3 Model Segmentation

WASP6.1 model segmentation was achieved with the use of an external hydrodynamic linkage file created with DYNHYD5. The linkage file was imported into the WASP6.1 preprocessor, and the DYNHYD5 junction to WASP6.1 segment map, provided in Table 4.7, automatically defined the segments within the model network. Figure 4.4 below is an ArcView location plot of the segment network used in model calibration, validation, and sensitivity analysis.

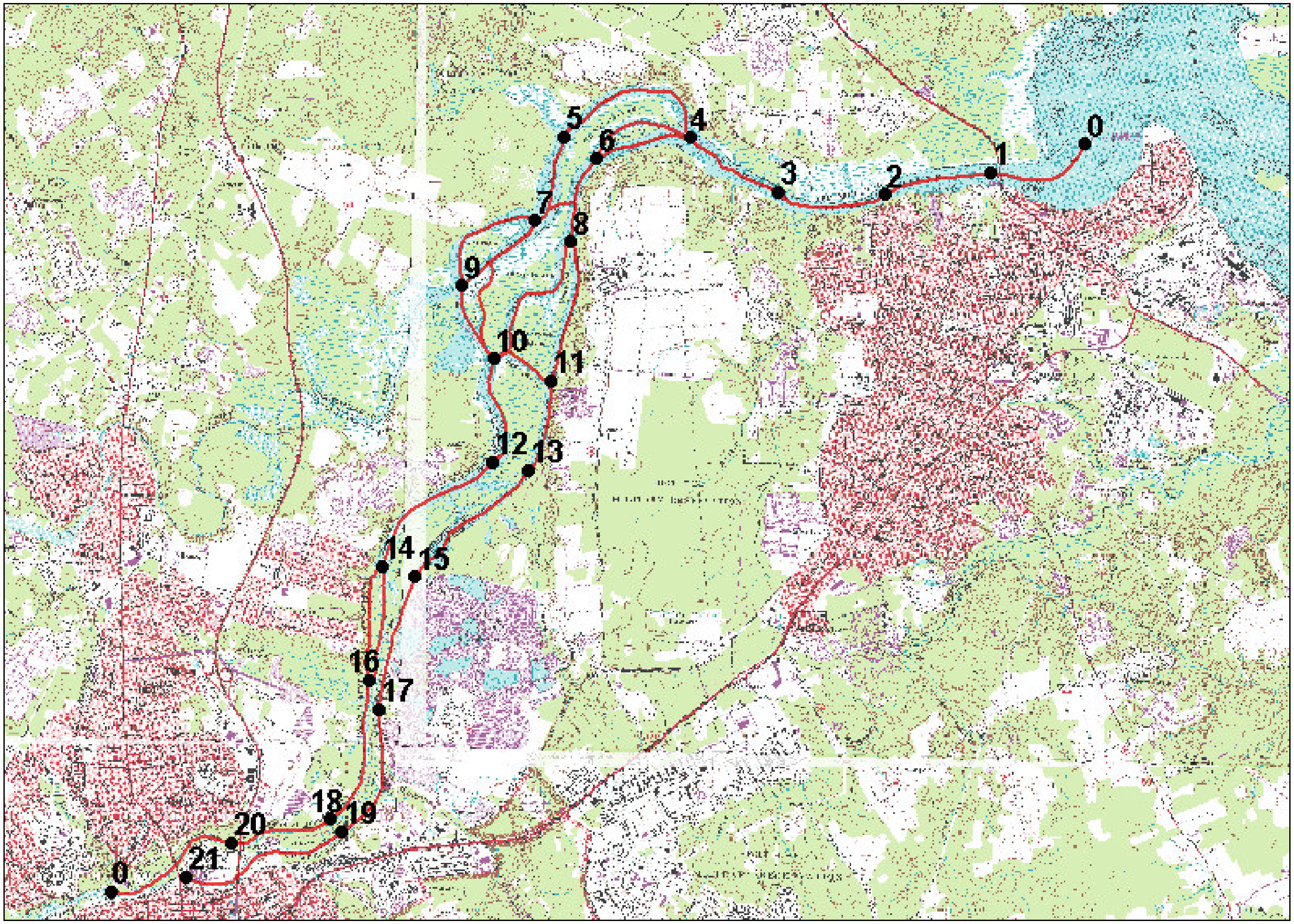

Figure 4.4 ArcView Plot of WASP6.1 Segment Network

Initial segment volumes, velocities, and depths were automatically defined with the hydrodynamic linkage file. In addition, they are updated by WASP6.1 at every time step using the remaining data stored within the linkage file. Initial WASP6.1 segment volumes, velocities, and depths are shown in Table 4.8.

Table 4.8 WASP6.1 Initial Segment Parameters

Segment Number	Volume (m^3)	Velocity (m/s)	Depth (m)
1	2240000	0.0000	3.6230
2	665000	0.0000	3.0999
3	725000	0.0000	2.8391
4	1220000	0.0000	2.3814
5	838000	0.0000	2.5316
6	404000	0.0000	1.6927
7	810000	0.0000	2.1088
8	325000	0.0000	1.0900
9	278000	0.0001	1.5989
10	435000	0.0000	1.2741
11	253000	0.0000	1.1690
12	397000	0.0000	1.3568
13	213000	0.0000	1.0375
14	220000	0.0000	1.1992
15	57500	0.0000	0.7546
16	127000	0.0000	0.8868
17	36800	0.0000	0.3700
18	30100	0.0000	0.5988
19	46700	0.0000	0.3700
20	29500	0.0020	0.3819
21	27400	0.0000	0.3700

A number of additional model parameters are also specified within the segments preprocessor screen. Segment water temperatures were held constant at 20°C, therefore, eliminating all temperature effects on fecal coliform die-off. In addition, segment initial fecal coliform (nitrate nitrogen) concentrations remained unchanged from the default setting of 0.00 cfu/100mL. HSPF water quality simulations were performed assuming that fecal coliform concentrations were 100% within the dissolved phase. Therefore, the fraction dissolved was not changed from the default value of 1.00.

4.4.4 Model Constants

Model constants such as coliform die-off rate at 20°C (denitrification rate at 20°C) and the temperature correction coefficient (denitrification temperature coefficient) were specified within this section of the WASP6.1 preprocessor. In order to develop base line fecal coliform concentrations for parameter sensitivity analysis, the coliform die-off rate was set to 0.2 day^{-1}. However, the temperature correction coefficient was not applied because segment water temperatures were held constant at 20°C.

4.4.5 Model Exchanges

As noted previously, when using 1-dimensional water quality models of estuaries, the mixing effects due to dispersion are typically much greater than the mixing effects due to diffusion (Martin and McCutcheon, 1999). As a result, the diffusion-mixing coefficient (E_x) in the advection-diffusion equation is replaced with a dispersion-mixing coefficient that carries the same units (m^2/s). Therefore, 3 different dispersion exchange functions (Appomattox Main Stem, Appomattox Canal, and Appomattox Branching) were defined with the aid of the WASP6.1 preprocessor. Within each exchange function, model segments were paired together denoting their linkage, and their interfacial mixing area (m^2) and characteristic mixing length (m) were specified. For this research, the interfacial mixing area between segments was assumed to be the channel cross-section area connecting the upstream and downstream segments. Channel cross-section areas are computed by DYNHYD5 and are printed within the DYNHYD5 output file (OUT file extension). Characteristic mixing lengths were assumed to be distance from upstream segment center to downstream segment center, which is also the length of the connecting channel. Channel lengths are readily obtained from the DYNHYD5 input file. Also, a constant dispersion coefficient (m^2/s) was defined for each exchange function. The parameters utilized to define each dispersive exchange function for WASP6.1 sensitivity analysis are presented below in Table 4.9 through 4.11.

Table 4.9 Appomattox Main Stem Dispersive Exchange Parameters

Downstream Segment	Upstream Segment	Mixing Area (m^2)	Mixing Length (m)	Dispersion Coefficient (m^2/s)
Boundary	1	2527.00	1298.00	1.00
1	2	672.00	1282.00	1.00
2	3	427.00	1317.00	1.00
3	4	514.00	1257.00	1.00
4	5	358.00	2060.00	1.00
5	7	598.00	1095.00	1.00
7	9	202.00	1461.00	1.00
9	10	114.00	959.00	1.00
10	12	175.00	1342.00	1.00
12	14	93.00	1867.00	1.00
14	16	26.00	1390.00	1.00
16	18	34.00	1774.00	1.00
18	20	22.00	1244.00	1.00
20	Boundary	31.00	1760.00	1.00

Table 4.10 Appomattox Canal Dispersive Exchange Parameters

Downstream Segment	Upstream Segment	Mixing Area (m^2)	Mixing Length (m)	Dispersion Coefficient (m^2/s)
4	6	305.00	1151.00	1.00
6	8	143.00	1071.00	1.00
8	11	115.00	1698.00	1.00
11	13	101.00	1096.00	1.00
13	15	60.00	1885.00	1.00
15	17	17.00	1617.00	1.00
17	19	32.00	1623.00	1.00
19	21	37.00	2047.00	1.00

Table 4.11 Appomattox Branching Dispersive Exchange Parameters

Downstream Segment	Upstream Segment	Mixing Area (m^2)	Mixing Length (m)	Dispersion Coefficient (m^2/s)
4	6	250.00	1329.00	1.00
6	7	6.00	1121.00	1.00
7	9	213.00	1159.00	1.00
7	10	17.00	1963.00	1.00
8	10	122.00	1885.00	1.00
10	11	28.00	853.00	1.00
14	16	18.00	1409.00	1.00

4.4.6 Model Loading Rates

MapTech, Inc. of Blacksburg, Virginia also developed a calibrated and validated HSPF water quality model of the Appomattox River basin. Time-variable, hourly-averaged (per day), HSPF loadings (1000 cfu/day) were used as inputs to the WASP6.1 model network. More specifically, segments 1 through 20 received 211 (January 1, 2003 through July 31, 2003) time-variable, hourly-averaged, HSPF coliform loadings, which account for both instream and overland loadings where necessary. WASP6.1 segments 5 (Ashton Creek), 9 (Swift Creek), and 16 (Oldtown Creek) receive inputs that account for both instream and overland coliform loadings. The remaining 17 WASP6.1 segments receive inputs that only account for overland coliform loadings. Due to the vast amount of data (4220 data points total), the time-variable coliform loadings rates will not be presented here. Model loading rates are contained within the WASP6.1 input data file, which can be obtained from the author of this document (Andrew Hammond, anhammo2@vt.edu).

A global conversion factor was applied to the time-variable coliform loading rates since the WASP6.1 nitrate nitrogen state variable was used to simulate fecal coliform bacteria. Within WASP6.1, nitrate loadings rates are specified with units of kg/day. Hard-coded (permanent) model conversion factors are used to produce model results (concentrations) with units of mg/L for nitrate. However, for this research fecal coliform concentrations with units of cfu/100mL are desirable as an end product. Therefore, a global conversion factor of 0.0001 was applied to all fecal coliform loadings, and model results were produced with units of cfu/100mL.

4.4.7 Model Boundary Concentrations

WASP6.1 requires the user to specify instream coliform concentrations (cfu/100mL) for all model boundaries. For this research 2 model boundaries were utilized. The upstream model boundary is located on the main stem of the Appomattox River upstream from model segment 20. The downstream model boundary is located at the confluence of the Appomattox and James Rivers downstream from model segment 1. Time-variable daily-averaged HSPF instream coliform concentrations (cfu/100mL) were used as the upstream boundary inputs. A sample of the time-variable boundary concentrations is presented below in Table 4.12. Upstream boundary concentrations are contained within the WASP6.1 input data file, which can be obtained from the author of this document (Andrew Hammond, anhammo2@vt.edu).

Table 4.12 Fecal Coliform Concentrations for Upstream WASP6.1 Boundary

Date	Time	Concentration (cfu/100mL)
1/1/03	1:00 AM	244.58
1/2/03	1:00 AM	332.41
1/3/03	1:00 AM	133.85
1/4/03	1:00 AM	273.22
1/5/03	1:00 AM	394.22
1/6/03	1:00 AM	262.96
1/7/03	1:00 AM	169.92
1/8/03	1:00 AM	113.56
1/9/03	1:00 AM	78.42
1/10/03	1:00 AM	56.52
1/11/03	1:00 AM	42.38
1/12/03	1:00 AM	33.43
1/13/03	1:00 AM	27.89
1/14/03	1:00 AM	24.32
1/15/03	1:00 AM	21.97

Downstream boundary concentrations utilized should be representative of fecal coliform concentrations within the James River since the downstream model boundary is located at the confluence of the Appomattox and James Rivers. The Virginia Department of Environmental Quality (VADEQ) has maintained a water quality sampling station (2JMS078.99) for fecal coliform and other pollutants at the intersection of the 2 rivers for the period of 1994 through 2001. A total of 83 instantaneous water quality samples were collected on an intermittent basis. Sampling periods range from bimonthly to monthly to every 7 months. As a result, a regular time-series of fecal coliform concentrations does not exist for use in this research. Therefore, a geometric average boundary concentration was established for each modeling period. Samples falling between October 1, 1998 and July 31, 2003 were used to determine a geometric average boundary concentration of 113 cfu/100mL for model calibration. Samples between October 1, 1993 and September 31, 1998 were utilized to calculate a geometric average boundary concentration of 254 cfu/100mL for model validation. A geometric average boundary concentration of 113 cfu/100mL (same as model calibration) was used for model sensitivity analysis since no samples existed for the 2003 calendar year. In addition, this geometric average downstream boundary concentration approach was the same utilized by the Delaware River Basin Commission (2003).

4.4.8 Model Time Step and Print Interval

When configuring DYNHYD5 to create an external hydrodynamic linkage file, the number of hydrodynamic time steps per water quality time step was specified as 30. As a result, this fixed the WASP6.1 time step to 900 sec (DYNHYD5's is 30 sec) or 15 minutes (expressed as 0.0104 days within WASP6.1). In addition, this time step combination of 30 sec and 15 minutes is the same utilized by the Delaware River Basin Commission (2003) for model development. A water quality time step of 15 minutes proved to be quite stable during sensitivity analysis, calibration, and validation simulation runs.

A model output print interval of 1 hour (0.0417 days) was chosen for this research. This corresponds directly to the output print interval chosen for HSPF water quality simulation runs. Since WASP6.1 calibration and validation runs are approximately 5 years in length, a significant amount of data is stored within the model output file (BMD file extension), and output file sizes tend to average around 200 MB. Therefore, hard drive capacity as well as model network size must be taken into consideration when selecting the model print interval.

4.5 Calibration and Validation of DYNHYD5 and WASP6.1

NOAA does not operate or maintain a tidal stage recorder at or near City Point, which serves as the downstream seaward boundary for the lower Appomattox River. Therefore, NOAA tide predictions for City Point were used as the seaward boundary condition for DYNHYD5 simulation runs. However, in order to calibrate and validate the hydrodynamic model, observed tidal heights at a location within the river system are required. Therefore, a stage recorder and data logger were installed at Hopewell City Marina, and water surface elevations were logged from May 22, 2003 to September 13, 2003, with a data gap from July 5, 2003 to August 8, 2003 due to a faulty battery. In addition, due to a lack of publicly available precipitation data, HSPF simulation runs were performed only from January 1, 1993 through July 31, 2003. Therefore, instream and overland flow inputs for DYNHYD5 could only be obtained during that time period. As a result, the time period from May 22, 2003 to July 5, 2003 was used for DYNHYD5 calibration and validation. The calibration time period selected was May 22, 2003 through June 13, 2003. In addition, the validation time period utilized was June 14, 2003 through July 5, 2003.

VADEQ maintains a water quality sampling point (2APP001.53) at the Route 10 bridge, which crosses the Appomattox River near Hopewell City Marina. At this location, VADEQ collects water quality samples to be tested for a number of different constituents, including fecal coliform bacteria. Long-term (1970 – present) records of coliform bacteria concentrations exist within VADEQ for this water quality sampling location. In addition, HSPF water quality simulation runs were performed from January 1, 1993 through July 31, 2003. Therefore, the calibration time period selected for WASP6.1 was October 1, 1998 through July 31, 2003. In addition, this is the same calibration period used for the calibration of HSPF. The validation time period selected was October 1, 1993 through September 30, 1998 and is the same time period used for HSPF validation.

4.5.1 DYNHYD5 Calibration and Validation

To calibrate the Appomattox River DYNHYD5 model, water surface elevations versus time were printed out for DYNHYD5 junction 2. In addition, it should be noted that the observed water surface elevations (logged with the pressure transducer and data collector at Hopewell City Marina) are located near the center of junction 2. Therefore, to perform model calibration, the simulated water surface elevations versus time were plotted against the observed water surface elevations versus time. Model parameters, such as channel roughness coefficient and tidal height scale, were modified until the simulated water surface elevations converged upon the observed water surface elevations. In addition, observed water surface elevations were plotted against simulated water surface elevations, and a linear regression analysis was utilized to produce a goodness-of-fit (r^2) value. As the r^2 value approaches 1.0, the simulated water surface elevations converge upon the observed water surface elevations.

After performing model calibration, the selected model parameters were validated using completely different input datasets (model inflows and tide predictions) and a different simulation time period. The simulated water surface elevations versus time were plotted against the observed water surface elevations versus time to verify convergence. In addition, a linear regression analysis was performed to once again verify goodness-of-fit.

DYNHYD5 calibration and validation results are presented in chapter 5 of this document. In addition, the aforementioned results are summarized in chapter 6.

4.5.2 WASP6.1 Calibration and Validation

WASP6.1 calibration and validation proceeded in the same manner as DYNHYD5 calibration and validation. However, instead of using water surface elevations for comparison at WASP6.1 segment 1 (DYNHYD5 junction 2), fecal coliform concentrations were utilized. For model calibration, simulated fecal coliform concentrations versus time were plotted against VADEQ observed fecal coliform concentrations, and model parameters, such as coliform die-off and dispersion coefficients, were varied until the two converged upon one another. Modeled concentrations were plotted against observed concentrations, and a linear regression analysis was performed to obtain a goodness-of-fit (r^2) value. The aforementioned procedure was also used to validate the selected WASP6.1 parameters.

The results of WASP6.1 calibration and validation are shown in chapter 5. They are summarized in chapter 6 of this document.

4.6 Model Sensitivity Analysis

Predetermined model inputs were varied by ±10% as well as ±50% to establish their impact on model results. Within DYNHYD5, a sensitivity analysis was performed on 4 different model inputs: tide predictions, streamflows, overland inflows, and Manning's roughness coefficients. Water surface elevations versus time were compared against pre-established base line values at 2 specific locations (junctions 2 and 13) within the DYNHYD5 model network. DYNHYD5 sensitivity analysis results are presented in chapter 5.

Within WASP6.1, a sensitivity analysis was also performed on 4 different model inputs: coliform boundary concentrations, coliform loading rates, coliform die-off rate, and dispersion coefficients. Fecal coliform concentrations versus time were compared against pre-determined base line values at 2 locations (segment 1 and segment 12) within the WASP6.1 model network. WASP6.1 sensitivity analysis results are shown in chapter 5 of this document.

For consistency, the time period selected for hydrodynamic and water quality sensitivity analysis was January 1, 2003 through July 31, 2003. In addition, input file generation for sensitivity analysis is presented and discussed in sections 4.3 and 4.4 of this chapter.

5.0 Model Results

The main objective of this research is to advance the process of improving water quality in the tidal Appomattox River through the implementation of a hydrodynamic model and water quality model that take into account the tidal effects present. To achieve this objective, DYNHYD5 coupled with WASP6.1 was selected as the modeling framework for this research from an array of candidate estuary hydrodynamic and water quality models. To successfully implement a hydrodynamic or water quality model, a sensitivity analysis must be performed on model input parameters to quantify their impact on model results such as water surface elevations or fecal coliform concentrations. The effects of tidal height, streamflow, overland flow, and Manning's roughness coefficient are quantified for DYNHYD5. In addition, the impacts of boundary concentration, loading rate, die-off rate, die-off temperature coefficient, and dispersion are quantified for WASP6.1. With the aid of the aforementioned sensitivity analysis, model input parameters are adjusted in order to calibrate DYNHYD5 and WASP6.1. Simulated water surface elevations are compared against observed water surface elevations for DYNHYD5 hydrodynamic calibration. In addition, modeled fecal coliform concentrations are compared with observed concentrations for WASP6.1 water quality calibration. As part of the validation of DYNHYD5 and WASP6.1 model parameters, simulation runs are performed for time periods not utilized in the calibration process, and model results are compared with observed values.

5.1 DYNHYD5 Model Results

Results obtained during DYNHYD5 sensitivity analysis, calibration, and validation are presented and discussed briefly in this section. Specific model input parameters were selected for analysis and their effects are quantified. In addition, modeled water surface elevations are compared against observed water surface elevations for DYNHYD5 calibration and validation.

5.1.1 Model Sensitivity Analysis

Tidal height, streamflow, overland flow, and Manning's roughness coefficient were selected as the model input parameters in which to perform a DYNHYD5 sensitivity analysis. These specific parameters were varied by ±10% as well as ±50% to quantify their impact on model results. Water surface elevation (WSEL) versus time was compared against pre-established base line values at 2 locations within the DYNHYD5 model network. Tables 5.1 and 5.2 below quantify the average percent change in water surface elevation within DYNHYD5 junctions 2 and 13 (shown in Figure 4.3) for each model parameter analyzed.

The time period selected for hydrodynamic model sensitivity analysis was January 1, 2003 through July 31, 2003. This time period encompasses the intervals utilized for model calibration and validation. Input file generation for DYNHYD5 sensitivity analysis is discussed in detail in chapter 4 of this document.

Table 5.1 Average % Change WSEL versus % Change in Parameter (Junction 2)

Model Parameter	+10% Parameter % Change WSEL	+50% Parameter % Change WSEL	-10% Parameter % Change WSEL	-50% Parameter % Change WSEL
Tidal Height	9.99	49.95	-9.98	Model Unstable
Overland Flow	0.00	0.00	0.00	0.00
Instream Flow	0.01	0.03	-0.01	-0.02
Manning' s Roughness	0.01	0.04	-0.01	-0.03

Table 5.2 Average % Change WSEL versus % Change in Parameter (Junction 13)

Model Parameter	+10% Parameter % Change WSEL	+50% Parameter % Change WSEL	-10% Parameter % Change WSEL	-50% Parameter % Change WSEL
Tidal Height	7.00	40.49	-5.59	Model Unstable
Overland Flow	0.01	0.03	-0.01	-0.03
Instream Flow	0.75	3.76	-0.75	-3.72
Manning' s Roughness	0.84	4.08	-0.85	-4.29

It should be noted that the average percent changes in water surface elevation shown in Tables 5.1 and 5.2 were calculated as an average of the instantaneous time-variable percent change in water surface elevation for each model parameter. The instantaneous time-variable percent changes in water surface elevation due to percent change in model input parameter are shown below in Figures 5.1 through 5.4 for DYNHYD junctions 2 and 13.

As shown in Tables 5.1 and 5.2 above, tidal heights (seaward boundary tide predictions) have the largest impact on modeled water surface elevations both downstream (junction 2) and upstream (junction 13). The percent change in water surface elevation versus percent change in boundary tidal height remains approximately constant throughout the entire simulation period for the downstream portion of the model network. This is reflected in Figures 5.1a and 5.1b. However, this not the case for the upstream portion of the model network. The percent change in water surface elevation versus percent change in tidal heights varies with time throughout the simulation time period. In addition, the percent change in water surface elevation approaches zero during time period of wet weather (such as January 22, 2003, April 12, 2003, and May 29, 2003). As a result, tidal heights (tide predictions) have a large impact on downstream model results during dry and wet weather; however, they only affect upstream model results during period of dry weather.

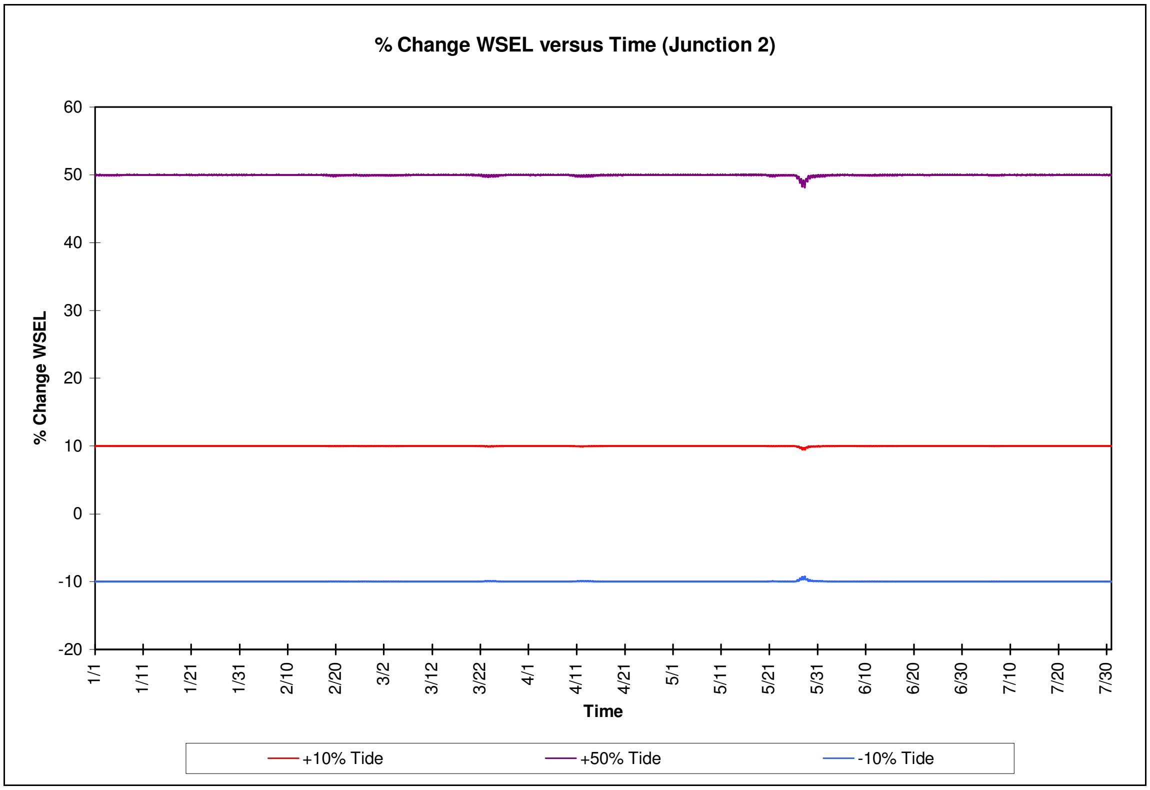

Figure 5.1a % Change WSEL versus % Change Tidal Height – Junction 2

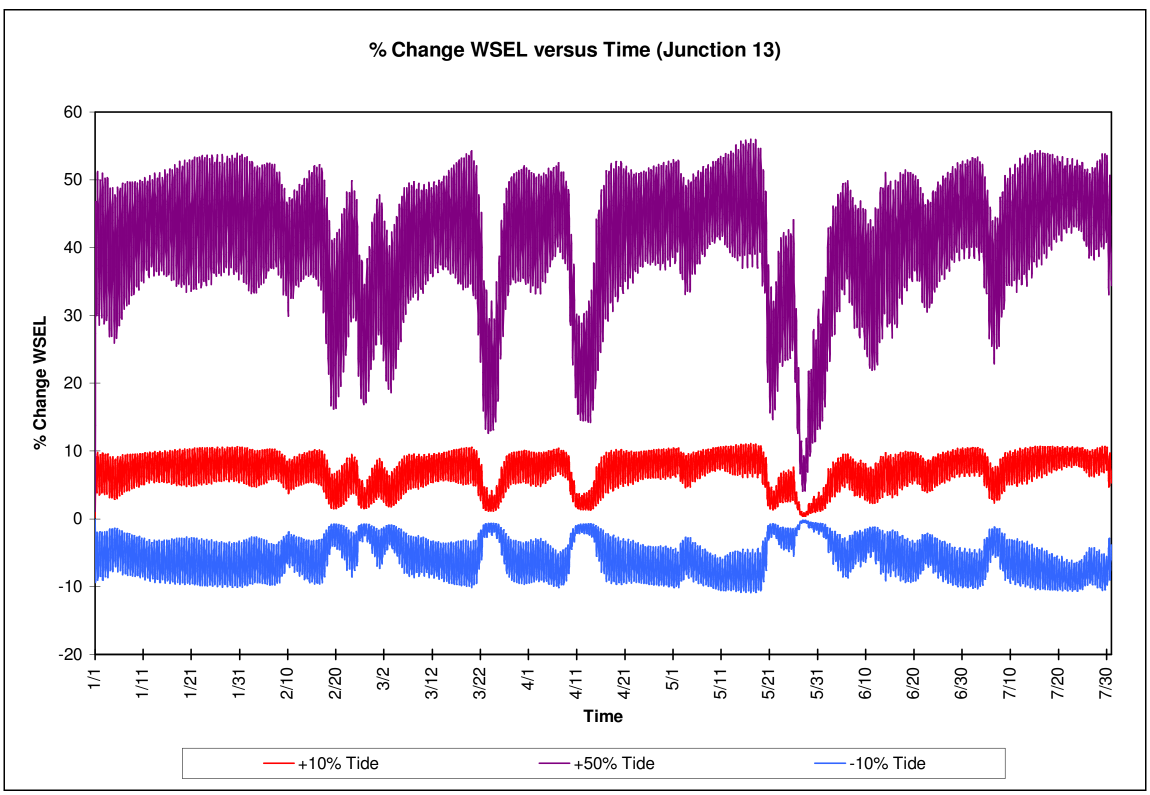

Figure 5.1b % Change WSEL versus % Change Tidal Height – Junction 13

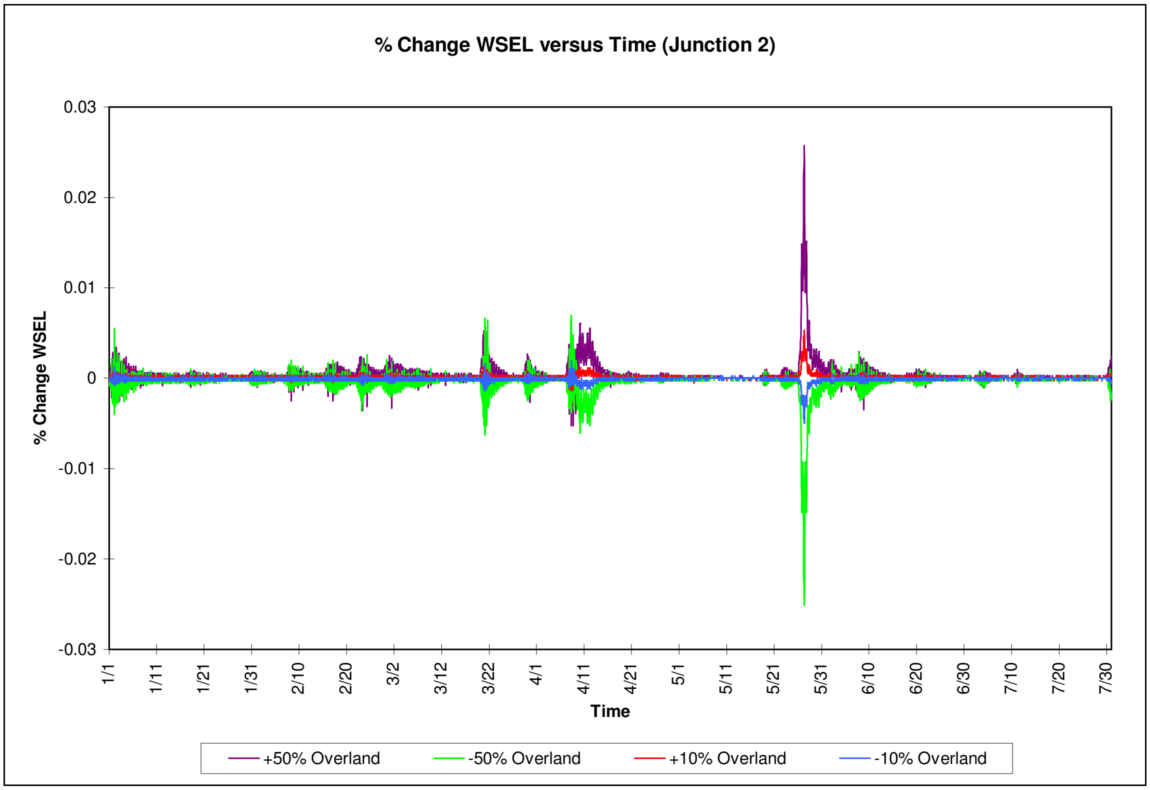

Figure 5.2a % Change WSEL versus % Change Overland Flow – Junction 2

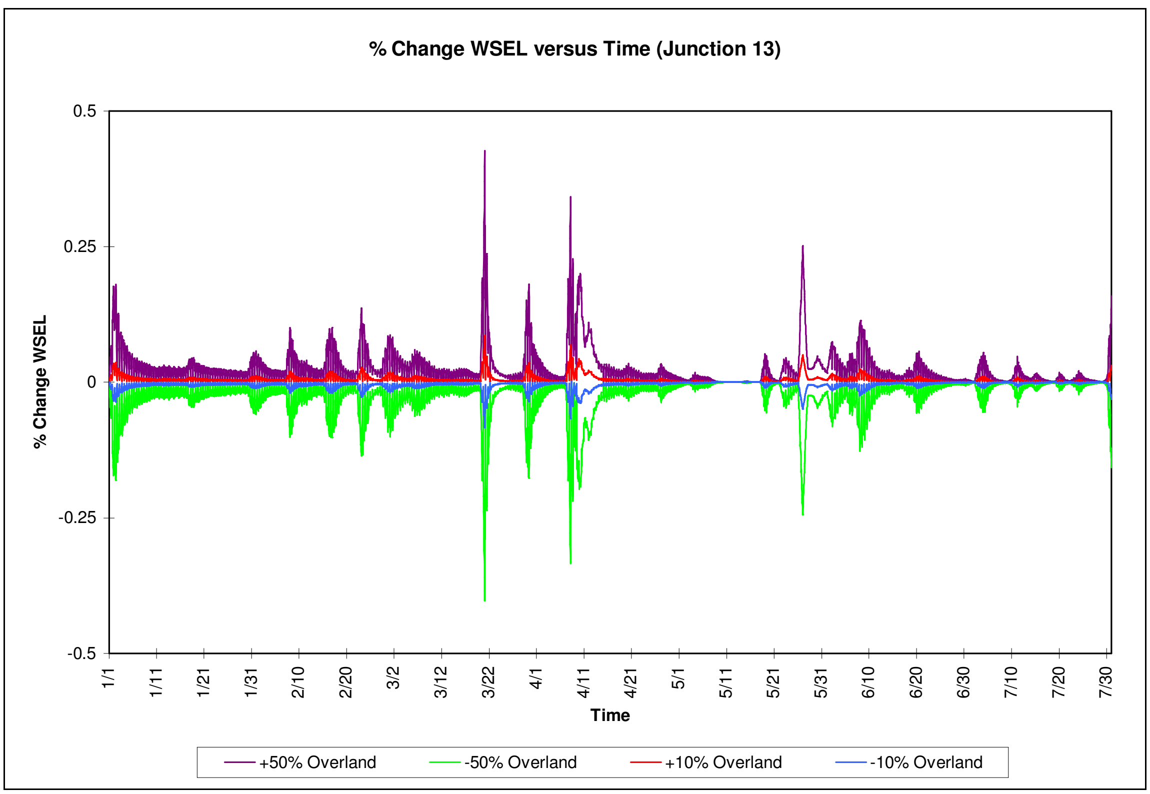

Figure 5.2b % Change WSEL versus % Change Overland Flow – Junction 13

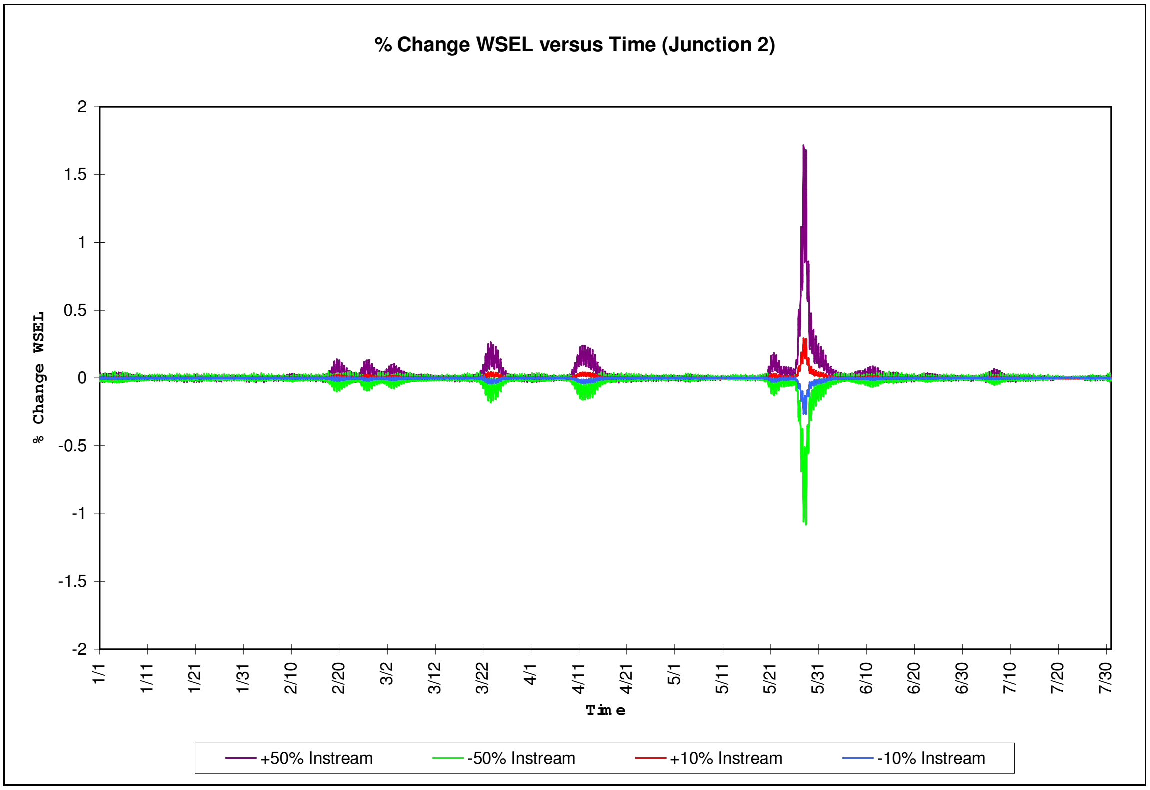

Figure 5.3a % Change WSEL versus % Change Instream Flow – Junction 2

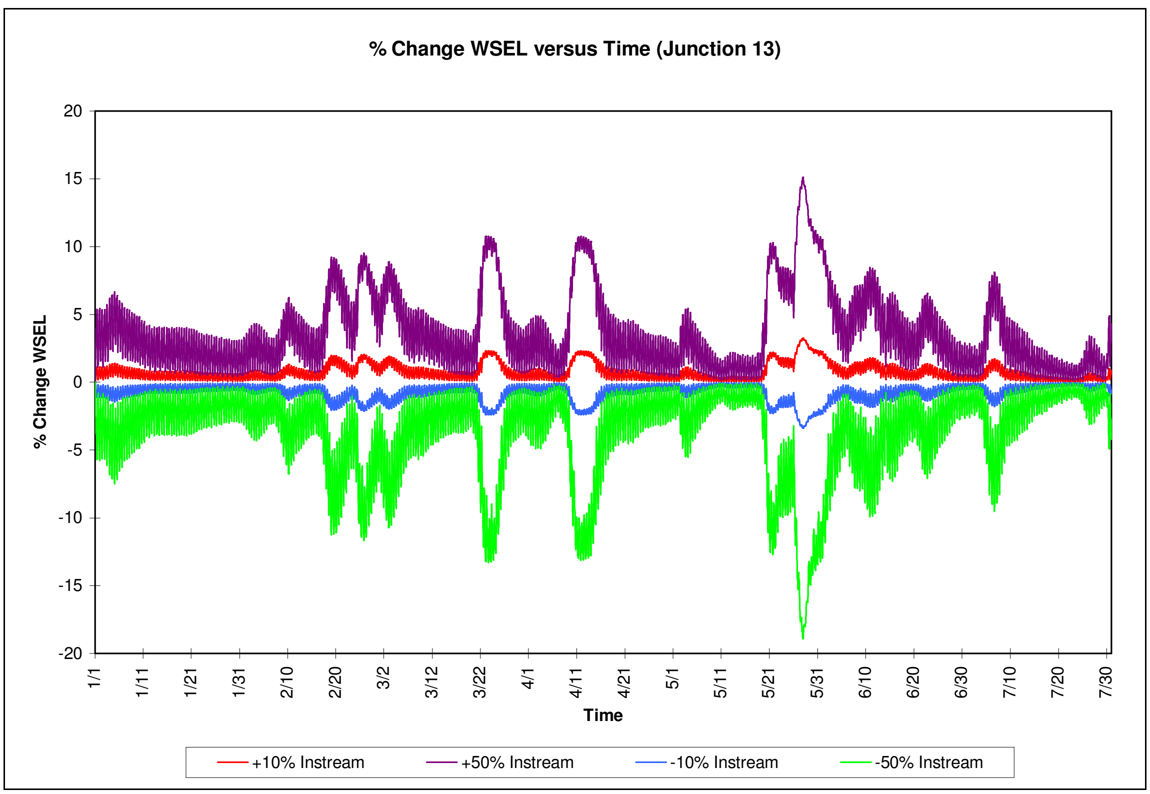

Figure 5.3b % Change WSEL versus % Change Instream Flow – Junction 13

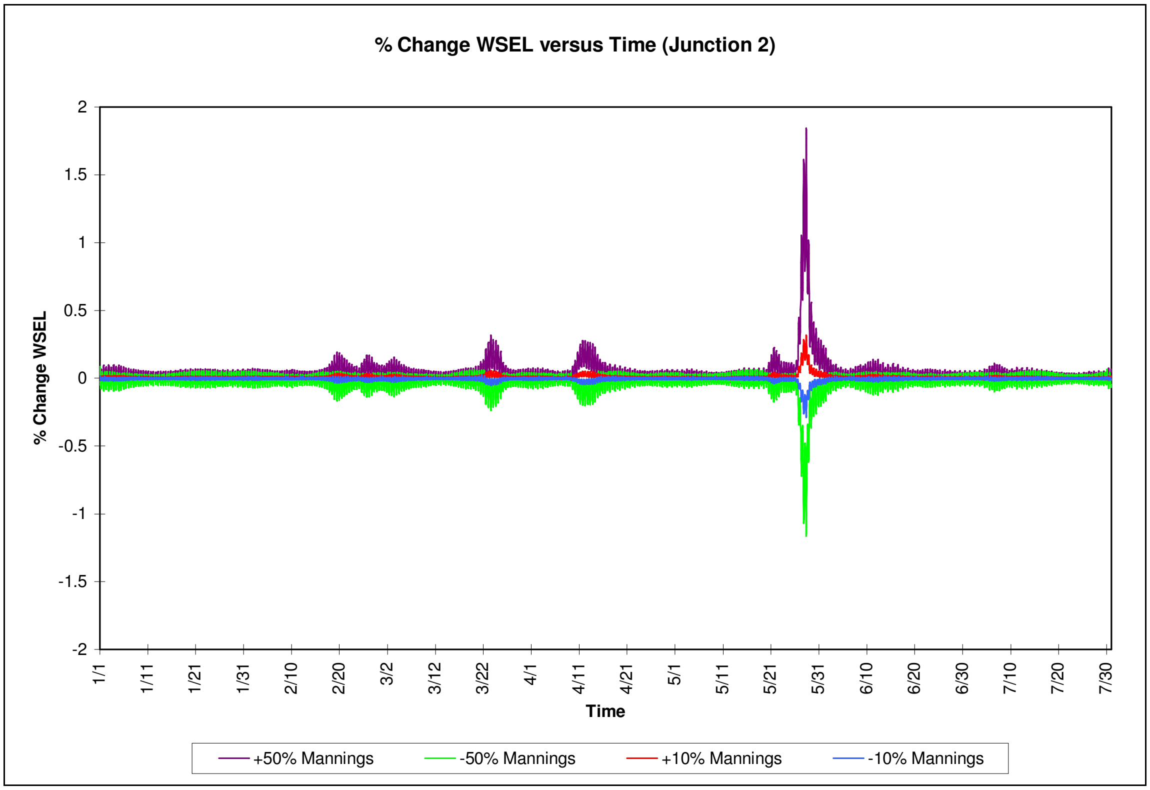

Figure 5.4a % Change WSEL versus % Change Manning's Coeff. – Junction 2

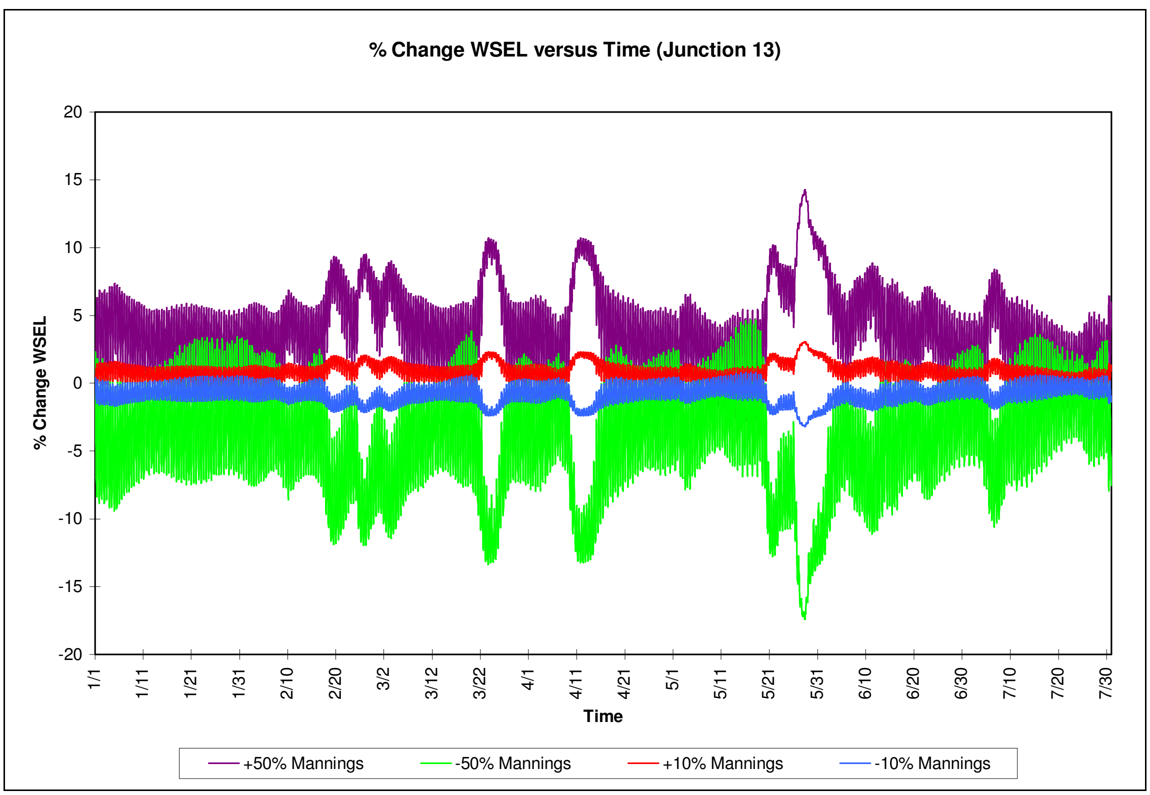

Figure 5.4b % Change WSEL versus % Change Manning's Coeff. – Junction 13

Overland inflows have the smallest impact on modeled water surface elevations both downstream and upstream. As shown in Tables 5.1 and 5.2 as well as Figures 5.2a and 5.2b, overland inflows do not significantly affect modeled water surface elevations throughout the simulation period. As a result, the time-variable overland inflows utilized during DYNHYD5 sensitivity analysis were replaced with average overland inflows for model calibration and validation. In addition, average overland inflows were utilized when creating external hydrodynamic linkage files for WASP6.1 sensitivity analysis, calibration, and validation. The time-variable overland inflow replacement procedure is explained in further detail in chapter 4.

The results obtained during model sensitivity analysis were used to optimize DYNHYD5 input parameters throughout the model calibration process. Sensitivity analysis proved to be quite effective in lending insight to which model parameters to modify for more reasonable model results.

5.1.2 Model Calibration

The time period selected for hydrodynamic model calibration was May 22, 2003 through June 13, 2003. The selection of this simulation time period for model calibration is discussed in detail in chapter 3. In addition, this calibration time period falls within the time period utilized for DYNHYD5 sensitivity analysis. Input file generation for model calibration remains the same as model sensitivity analysis and is discussed in its entirety in chapter 4.

Calibration the lower Appomattox River hydrodynamic model involved comparing simulated water surface elevations versus time, as output by DYNHYD5 at model junction 2. Modeled water surface elevations versus time were compared with observed water surface elevations (logged with the pressure transducer and data collector at Hopewell City Marina) versus time. Model input parameters, such as channel roughness coefficient and tidal height scale, were modified or tweaked until the simulated water surface elevations converged upon the observed water surface elevations. Results obtained during DYNHYD5 sensitivity analysis were utilized to determine which model input parameters to modify for more reasonable DYNHYD5 results. In addition, modeled water surface elevations were plotted against observed water surface elevations, and a linear regression analysis was utilized to produce a goodness-of-fit (r^2) value. As the r^2 value approaches 1.0, the simulated water surface elevations converge upon the observed water surface elevations.

Figures 5.5a and 5.5b below serve as a graphical representation of the final DYNHYD5 model calibration. Modeled water surface elevations do not correspond exactly to the observed water surface elevations, which were recorded at Hopewell City Marina. This discrepancy may be attributed to the use of NOAA tide predictions at the downstream seaward boundary (confluence of Appomattox and James Rivers) instead of observed water surface elevations. Tide predictions are yearly forecasts and may not accurately represent the actual system. DYNHYD5 calibration results are summarized in further detail in chapter 6.

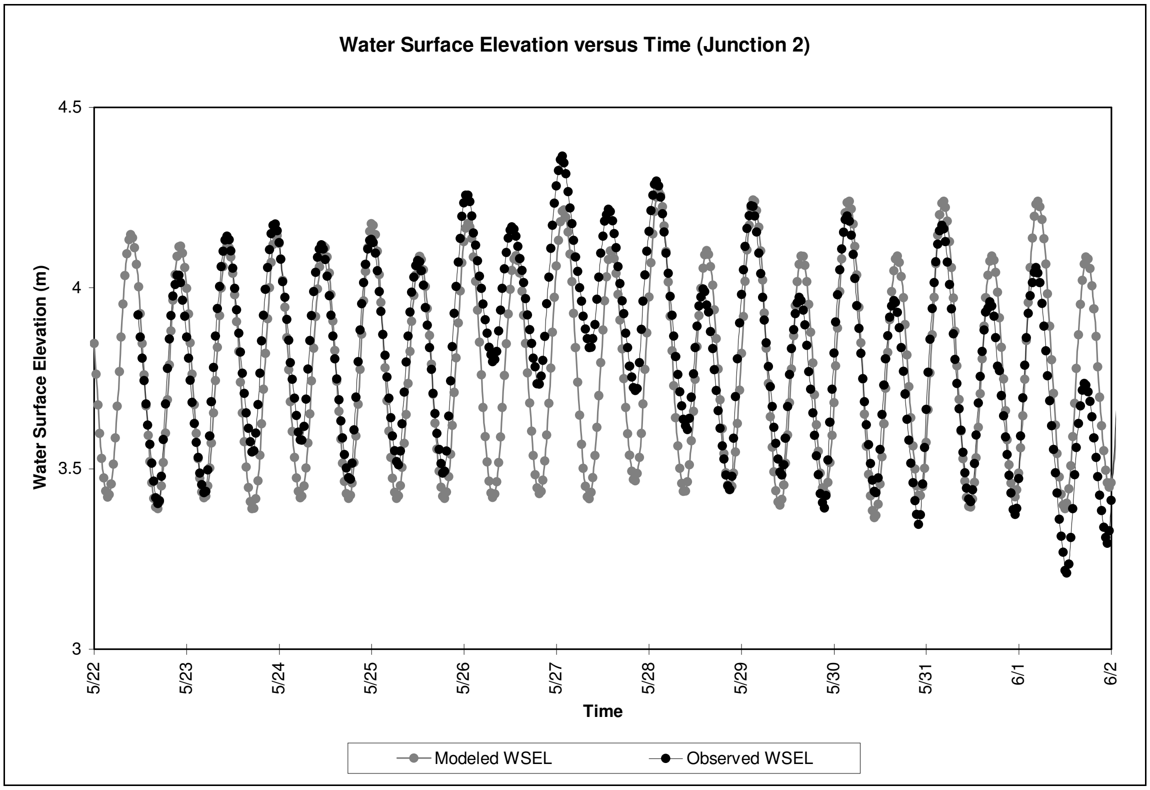

Figure 5.5a Modeled versus Observed WSEL for DYNHYD5 Calibration

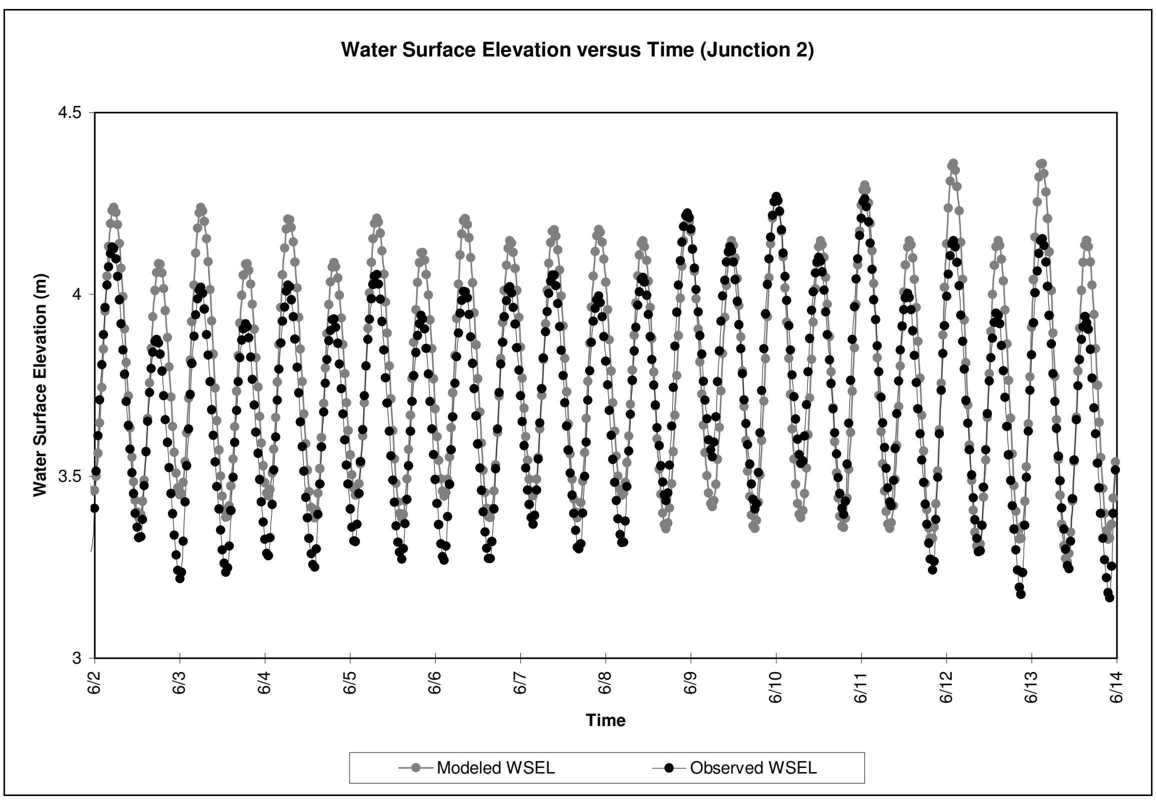

Figure 5.5b Modeled versus Observed WSEL for DYNHYD5 Calibration

Figure 5.6 below is a plot of modeled water surface elevation versus observed water surface elevation. After plotting the data, a linear regression was performed to determine a goodness-of-fit (r^2) value for DYNHYD5 calibration. As stated earlier, as the r^2 value approaches 1.0, the modeled water surface elevations converge upon the observed water surface elevations, which is the ultimate goal of model calibration in this research.

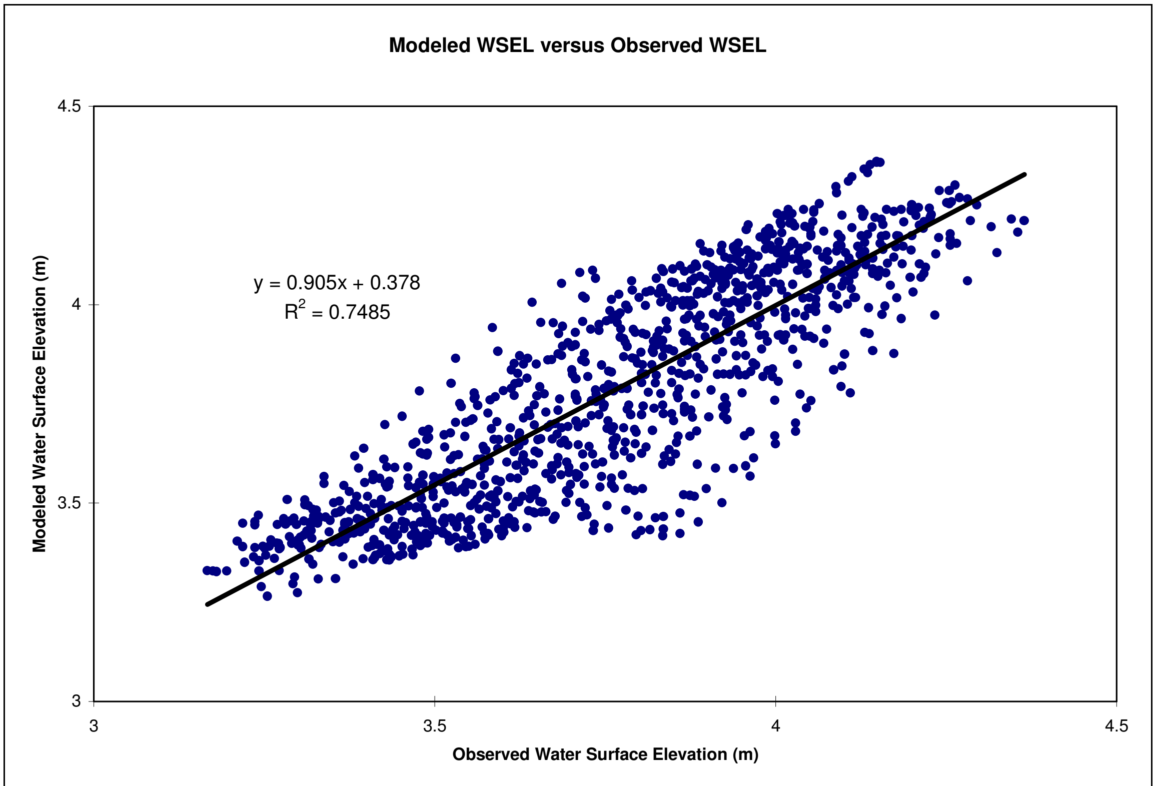

Figure 5.6 DYNHYD5 Calibration Goodness-of-Fit (r^2) Value Determination

As shown in Figure 5.6, a goodness-of-fit (r^2) value of 0.749 was obtained for DYNHYD5 calibration. As a result, modeled water surface elevations are not directly equivalent to observed water surface elevations, which was noted earlier in Figures 5.5a and 5.5b.

5.1.3 Model Validation

The time period selected for DYNHYD5 model validation was June 14, 2003 through July 5, 2003. The selection of this simulation time period for model validation is discussed in detail in chapter 4. In addition, this validation time period falls within the time period utilized for DYNHYD5 sensitivity analysis.

To validate the lower Appomattox River hydrodynamic model, modeled water surface elevations versus time were output by DYNHYD5 at model junction 2. Simulated water surface elevations were compared against observed water surface elevations to ensure the accuracy of model parameterization. Therefore, model input parameters remained unchanged during the validation process. Simulated water surface elevations were plotted against observed water surface elevations, and a linear regression analysis was utilized to produce a goodness-of-fit (r^2) value. This procedure is the same as that used during DYNHYD5 calibration.

Figures 5.7a and 5.7b below are a graphical representation of DYNHYD5 input parameter validation for the tidal Appomattox River. As expected, the simulated water surface elevations do not correspond exactly to the observed water surface elevations. The primary cause of discrepancy is believed to be the use of NOAA tide predictions at the downstream seaward boundary. As stated earlier, tide predictions are yearly forecasts and may not accurately represent the actual system. DYNHYD5 validation results are summarized in chapter 6.

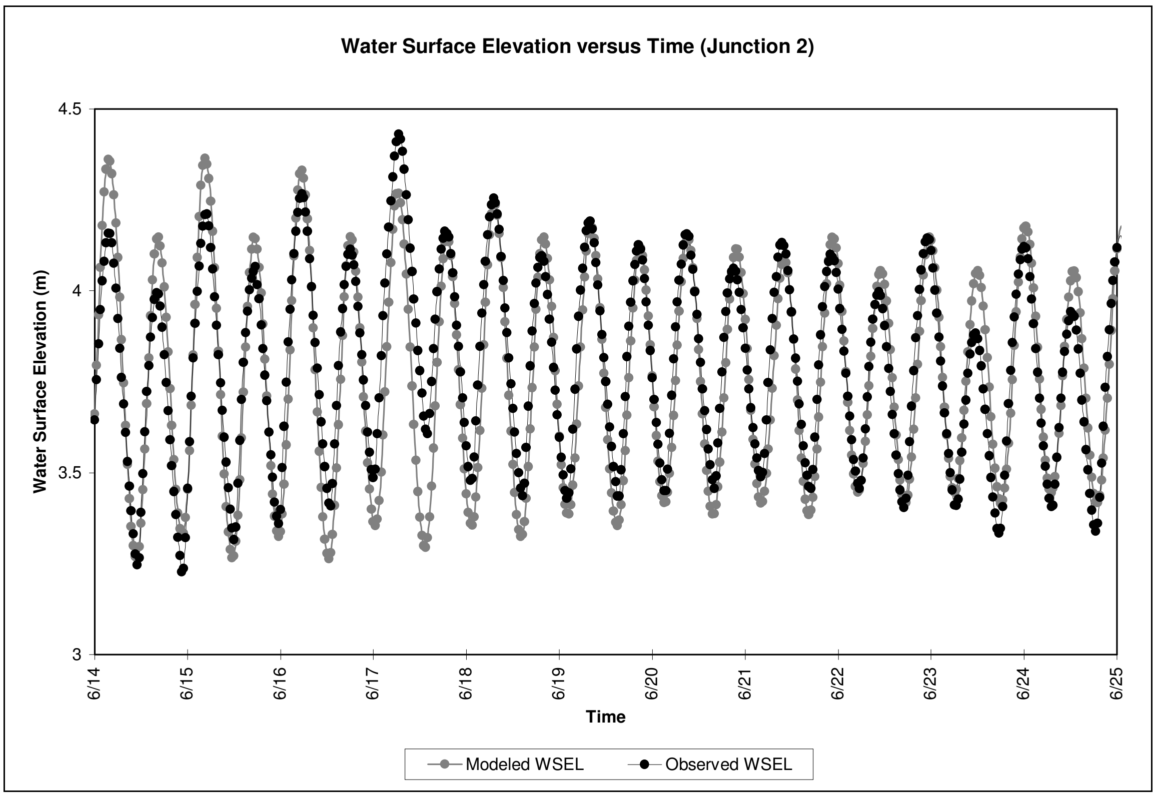

Figure 5.7a Modeled versus Observed WSEL for DYNHYD5 Validation

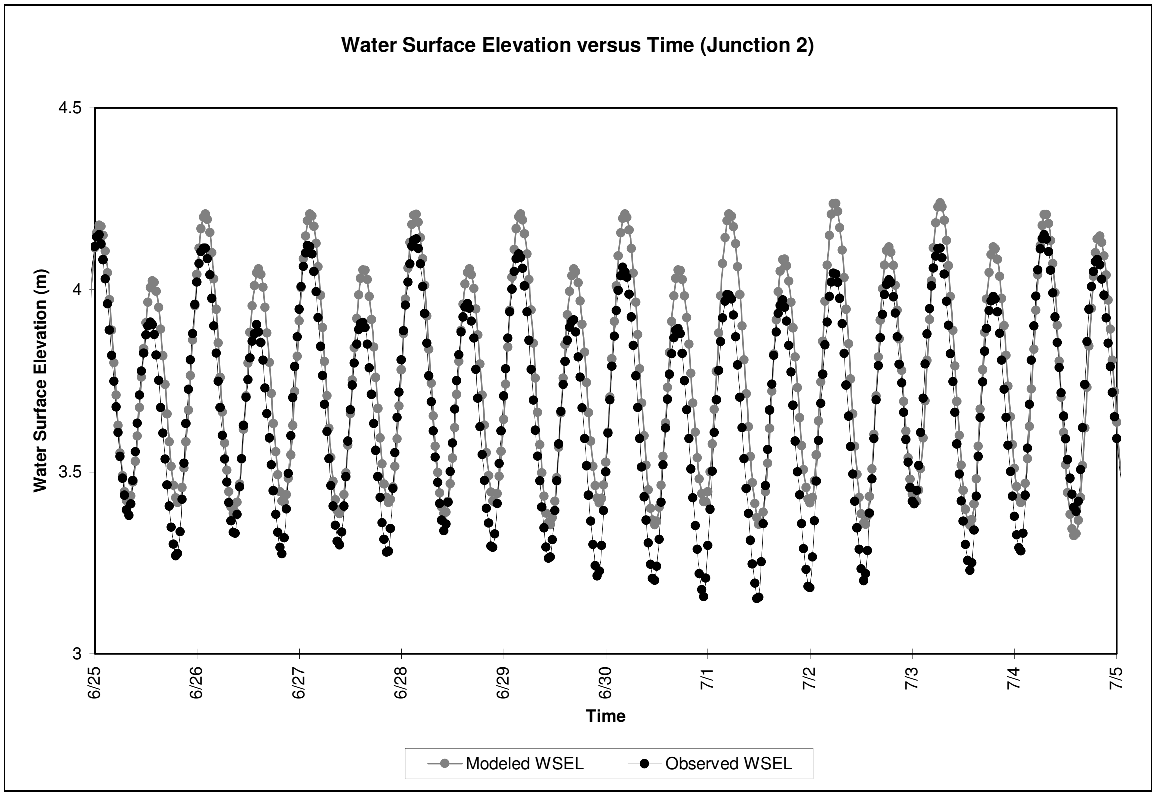

Figure 5.7b Modeled versus Observed WSEL for DYNHYD5 Validation

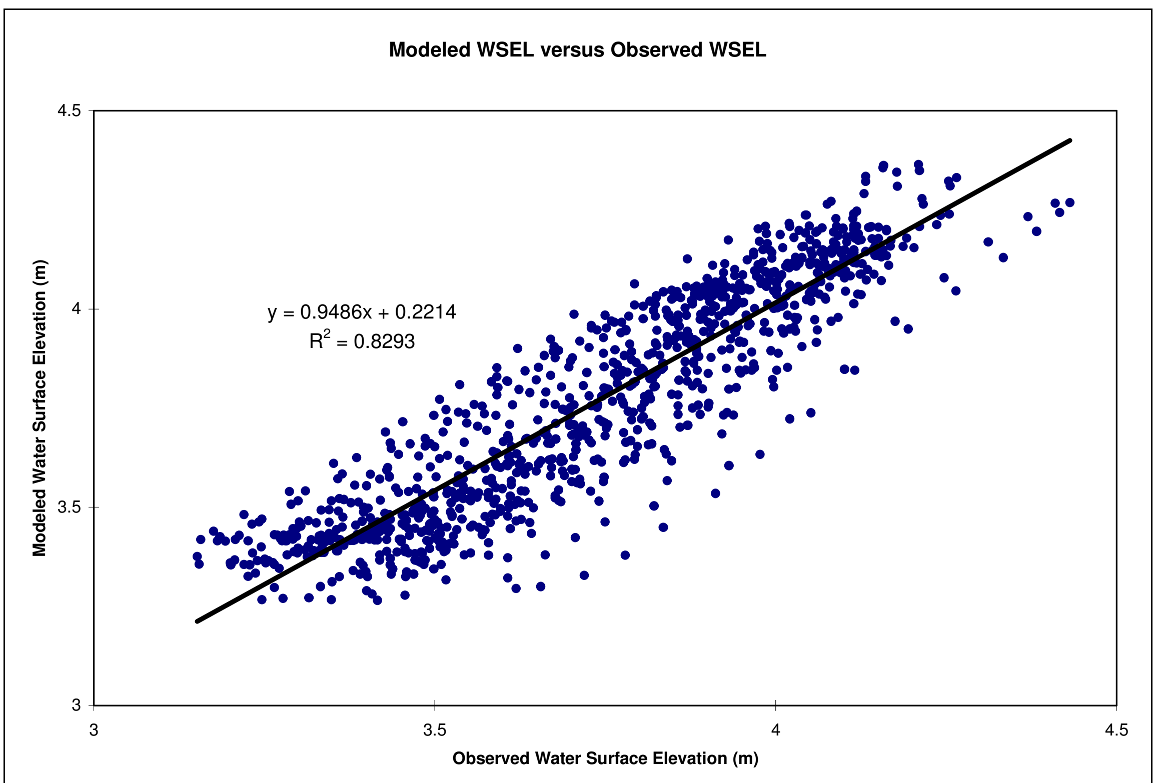

Figure 5.8 DYNHYD5 Validation Goodness-of-Fit (r^2) Value Determination

Figure 5.8 above is a plot of modeled water surface elevation versus observed water surface elevation. After plotting the data, a goodness-of-fit (r^2) value of 0.829 was calculated and is shown in the above figure. As a result, modeled water surface elevations are not directly equivalent to observed water surface elevations, which was noted earlier in Figures 5.7a and 5.7b.

One concern is the length of the time period used for model calibration and validation. Estuary hydrodynamic calibration and validation simulations are typically performed on the order of months to years. The time period used for DYNHYD5 calibration is 23 days in length, and the time period used for model parameter validation is 22 days in length. As a result, DYNHYD5 calibration and validation results were combined in order to determine a goodness-of-fit (r^2) value for the entire simulation time period (May 22, 2003 through July 5, 2003).

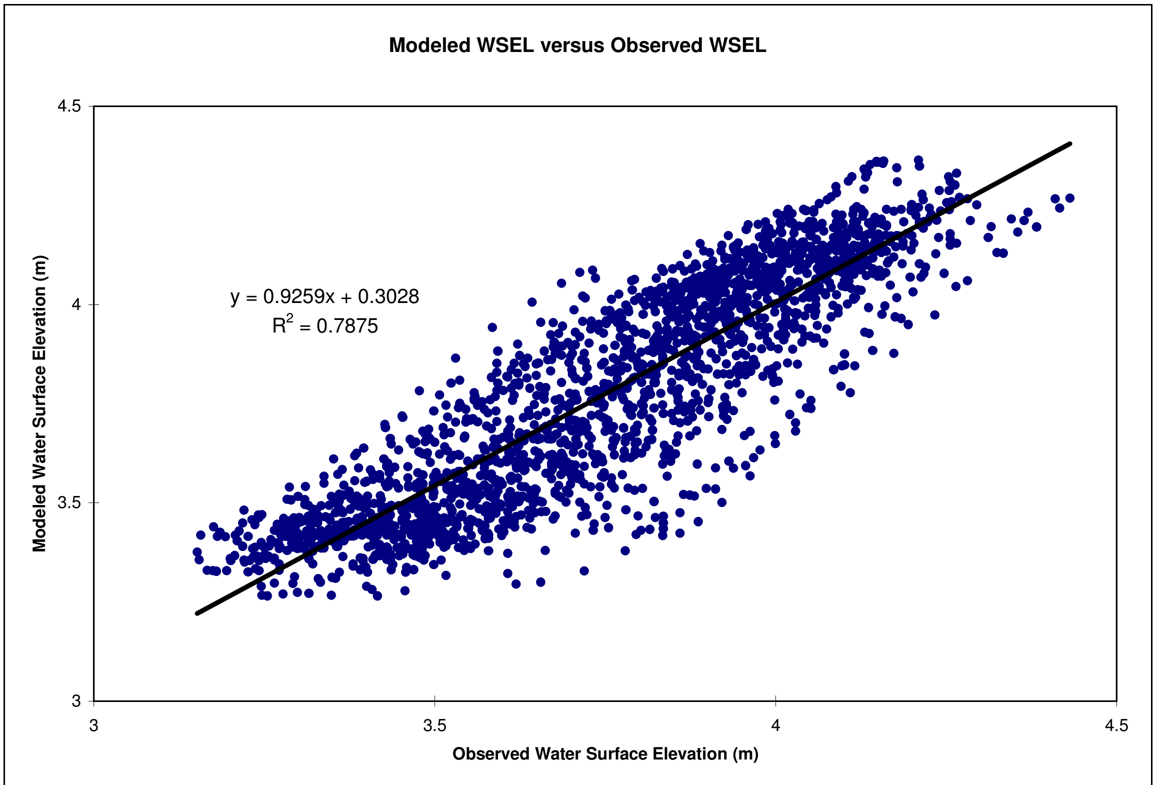

Figure 5.9 DYNHYD5 Goodness-of-Fit (r^2) Value Determination

Figure 5.9 above is a plot of modeled water surface elevation versus observed water surface elevation. As shown in the figure, the goodness-of-fit value for the entire simulation period is 0.788, which is also reflected in the data. Modeled water surface elevations do not correspond directly with observed water surface elevations, which is not uncommon in hydrodynamic modeling. As stated earlier, this discrepancy may be attributed to the use of NOAA tide predictions at the downstream seaward boundary instead of observed water surface elevations.

NOAA tide predictions (high and low water surface elevations) are typically separated in time by a period of 5 to 8 hours for the lower Appomattox River. Therefore, the NOAA tide predictions utilized for seaward boundary conditions do not correspond directly in time with the 30-minute pressure transducer data used for model calibration and validation. As a result, modeled high and low water surface elevations were compared against observed high and low water surface elevations. Linear regression analysis was utilized to determine a goodness-of-fit (r^2) values for model calibration and validation, as well as one for the entire DYNHYD5 simulation period (May 22, 2003 through July 5, 2003). A r^2 value of 0.874 was calculated for model calibration, 0.935 for model validation, and 0.904 for the entire simulation period. These calculated values emphasize the model's capability of reproducing high and low water surface elevations, which may prove to be critical during water quality simulations.

5.2 WASP6.1 Model Results

Results obtained during WASP6.1 sensitivity analysis, calibration, and validation are presented and discussed briefly in this section. Specific model input parameters were selected for analysis and their effects are quantified. In addition, modeled fecal coliform concentrations are compared against VADEQ observed fecal coliform concentrations for WASP6.1 calibration and validation.

5.2.1 Model Sensitivity Analysis

Boundary concentrations, loading rates, coliform die-off rate, and dispersion coefficients were selected as the model input parameters on which to perform a WASP6.1 sensitivity analysis. The aforementioned parameters were varied by ±10% as well as ±50% to quantify their significance on model results. Fecal coliform concentration versus time was compared against established baseline values at 2 locations within the WASP6.1 model network. Tables 5.3 and 5.4 below quantify the average percent change in fecal coliform concentration within WASP6.1 segments 1 and 12 (shown in Figure 4.4) for each model parameter analyzed.

The time period selected for water-quality model sensitivity analysis was January 1, 2003 through July 31, 2003. In addition, this time period encompasses the time period utilized for DYNHYD5 sensitivity analysis, calibration, and validation. Input file generation for WASP6.1 sensitivity analysis is discussed in detail in chapter 4.

Table 5.3 Average % Change Conc. versus % Change in Parameter (Segment 1)

Model Parameter	+10% Parameter % Change Conc.	+50% Parameter % Change Conc.	-10% Parameter % Change Conc.	-50% Parameter % Change Conc.
Boundary Conc.	2.38	11.91	-2.38	-11.91
Loading Rate	7.62	38.08	-7.62	-38.08
Die-off Rate	-3.20	-13.72	3.49	21.29
Dispersion	-0.11	-0.56	0.11	0.56

Table 5.4 Average % Change Conc. versus % Change in Parameter (Segment 12)

Model Parameter	"+10% Parameter" % Change Conc.	"+50% Parameter" % Change Conc.	"-10% Parameter" % Change Conc.	"-50% Parameter" % Change Conc.
Boundary Conc.	6.67	33.36	-6.67	-33.36
Loading Rate	3.33	16.63	-3.33	-16.63
Die-off Rate	-0.44	-2.15	0.45	2.32
Dispersion	0.01	0.06	-0.01	-0.06

It should be noted that the average percent changes in fecal coliform concentration shown in Tables 5.3 and 5.4 were calculated as an average of the instantaneous time-variable percent change in fecal coliform concentration for each model parameter. The instantaneous time-variable percent changes in fecal coliform concentration due to percent change in model input parameter are shown below in Figures 5.10 through 5.13 for WASP6.1 segments 1 and 12.

As shown in Table 5.3, fecal coliform bacteria loading rates have the largest impact on WASP6.1 modeled coliform concentrations for the downstream portion (segment 1) of the lower Appomattox River. The percent change in fecal coliform concentration follows a fairly regular pattern throughout the entire simulation period for the downstream portion of the model network. During periods of wet weather, the percent change in coliform concentration is approximately equal to the percent change in loading rate. However, during periods of normal or dry weather, the percent change in coliform concentration is typically lower than the percent change in loading rate. In addition, the percent change in coliform concentration due to change in loading rate occasionally approaches zero, which is shown in Figure 5.11a. Therefore, the adjustment of fecal coliform loading rates will have more of an impact on model results during periods of wet weather for the downstream portion of the WASP6.1 model network.

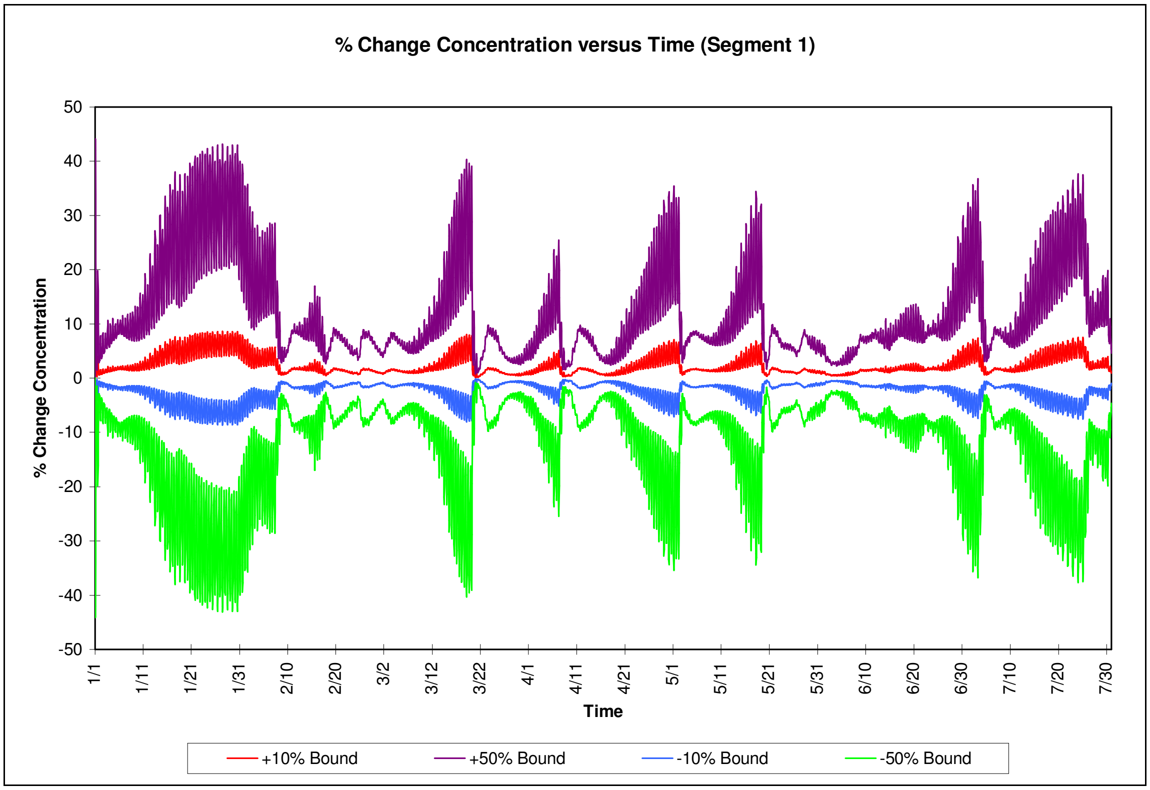

Figure 5.10a % Change Conc. versus % Change Boundary Conc. – Segment 1

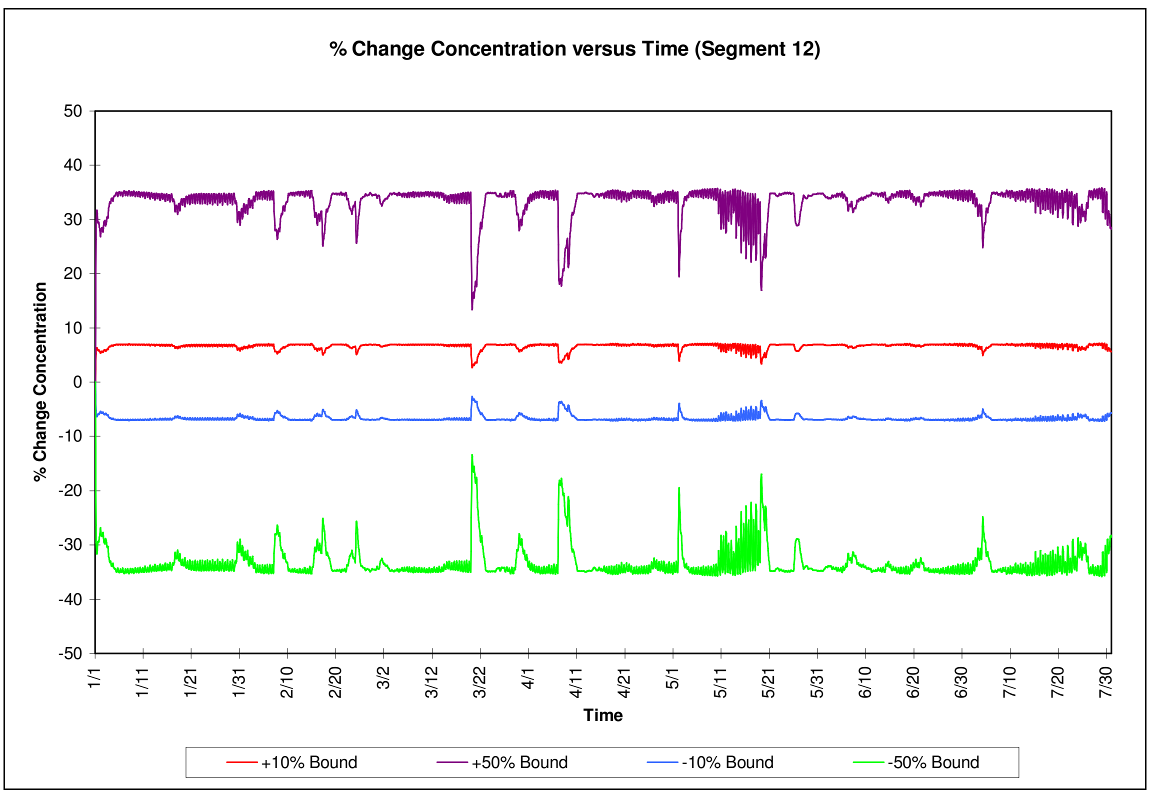

Figure 5.10b % Change Conc. versus % Change Boundary Conc. – Segment 12

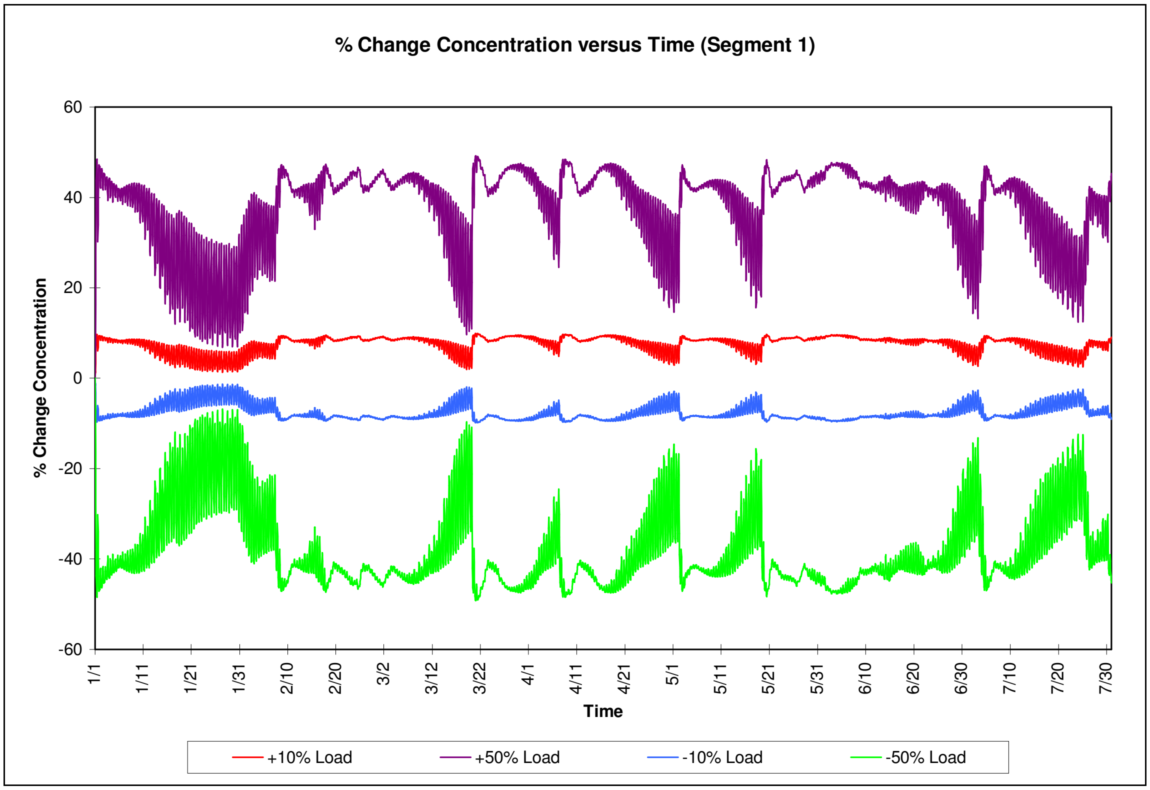

Figure 5.11a % Change Conc. versus % Change Loading Rate – Segment 1

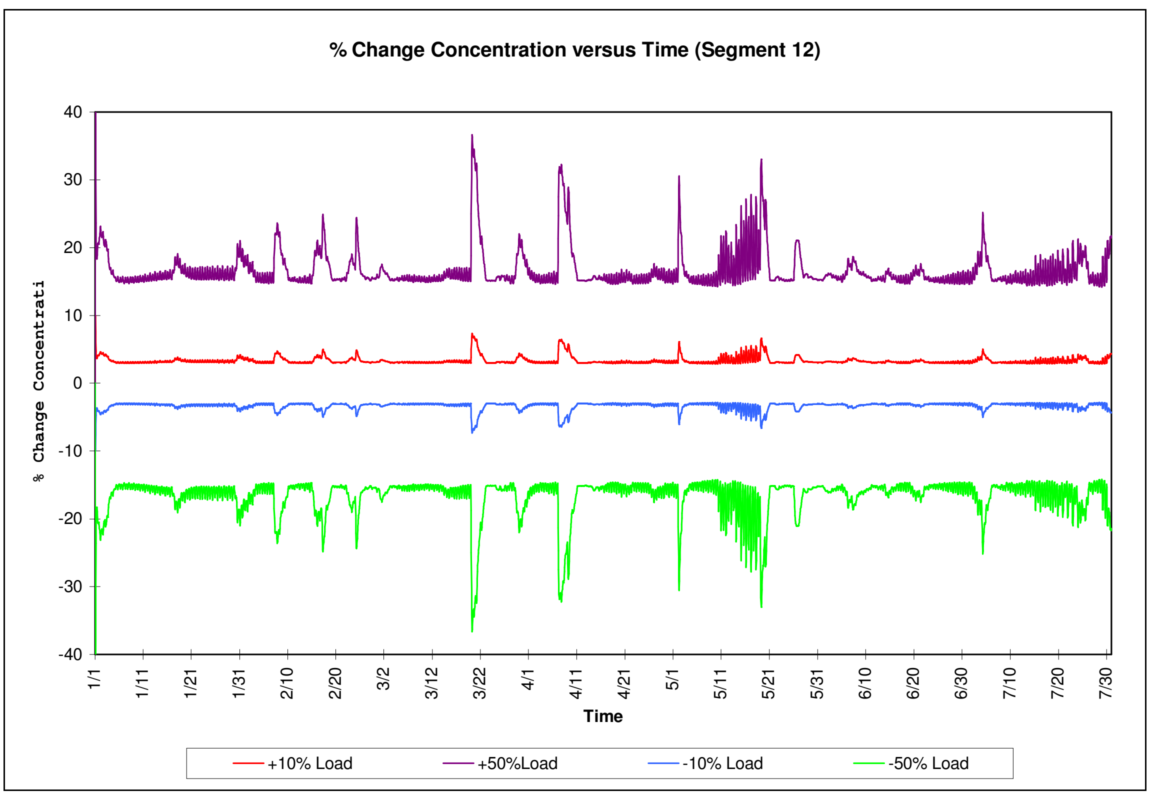

Figure 5.11b % Change Conc. versus % Change Loading Rate – Segment 12

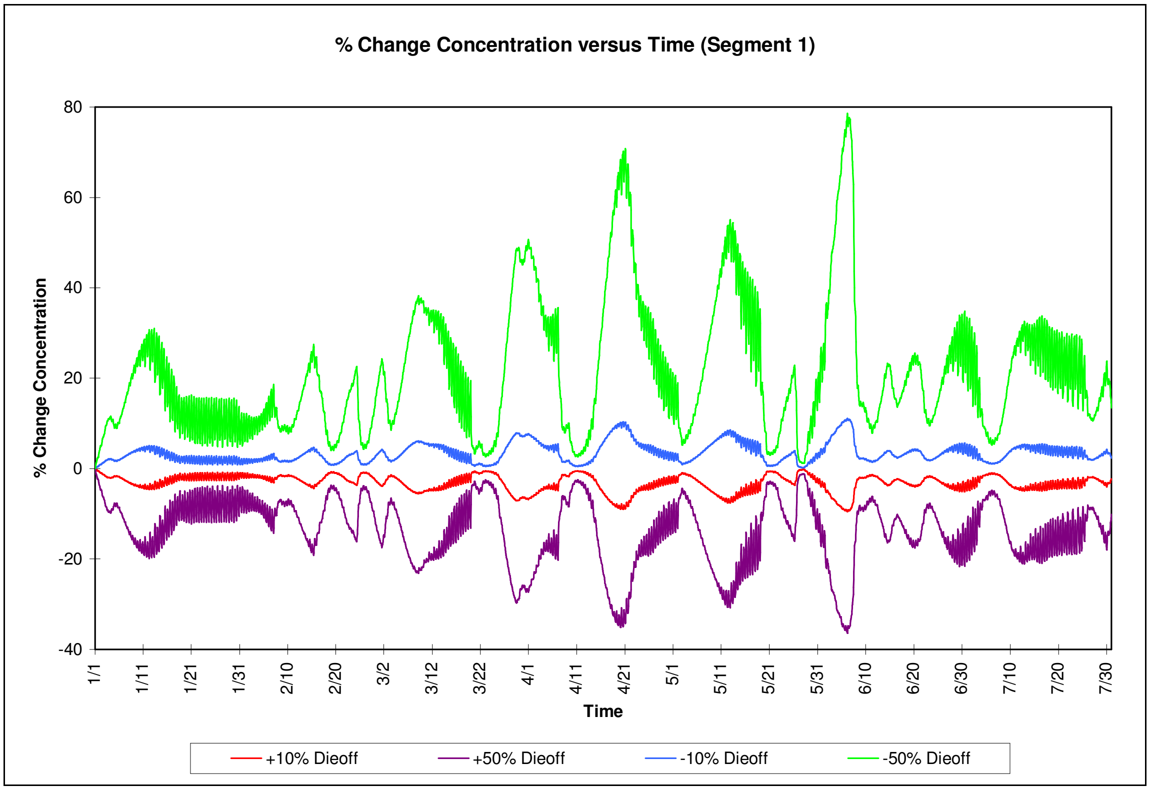

Figure 5.12a % Change Conc. versus % Change Die-off Rate – Segment 1

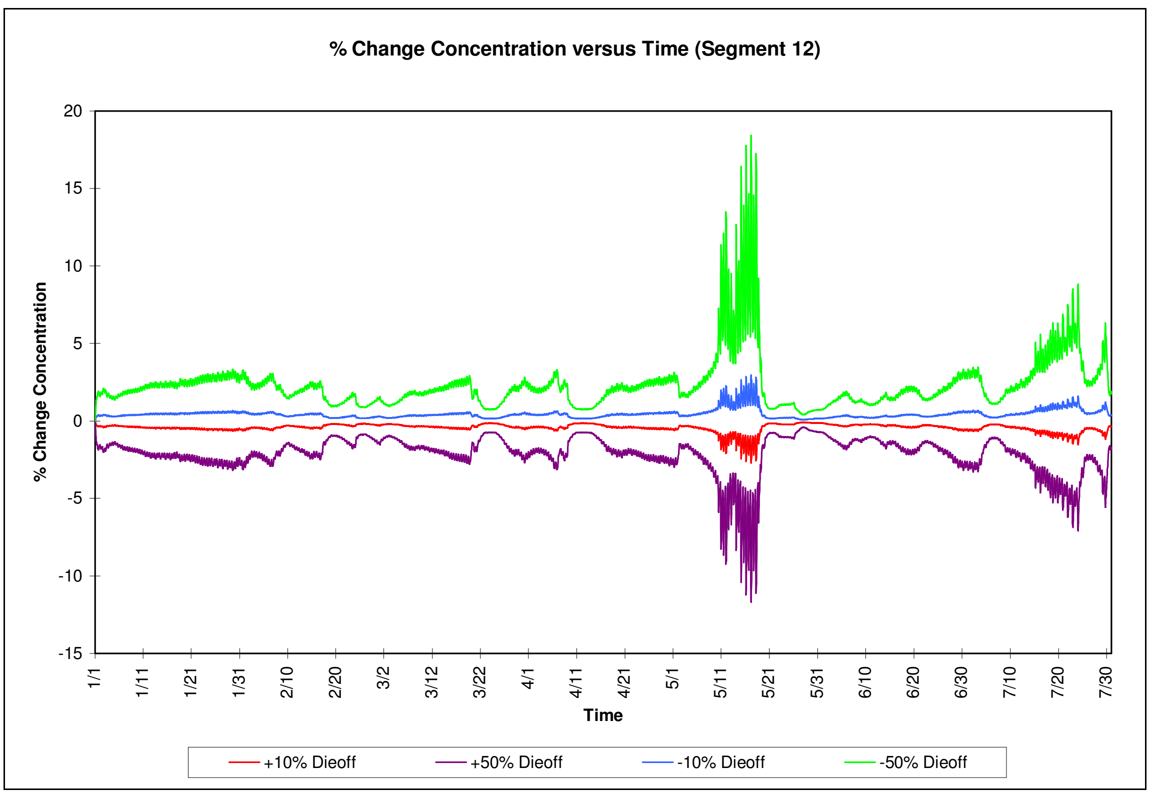

Figure 5.12b % Change Conc. versus % Change Die-off Rate – Segment 12

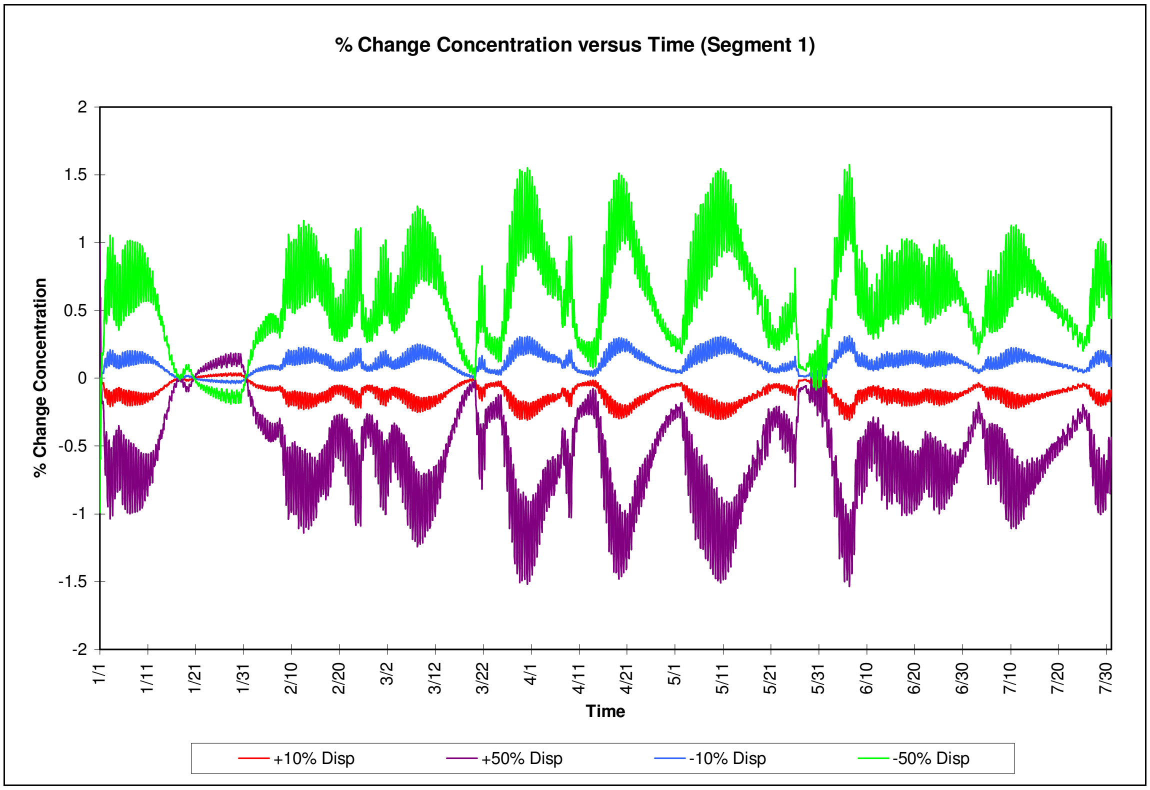

Figure 5.13a % Change Conc. versus % Change Dispersion Coeff. – Segment 1

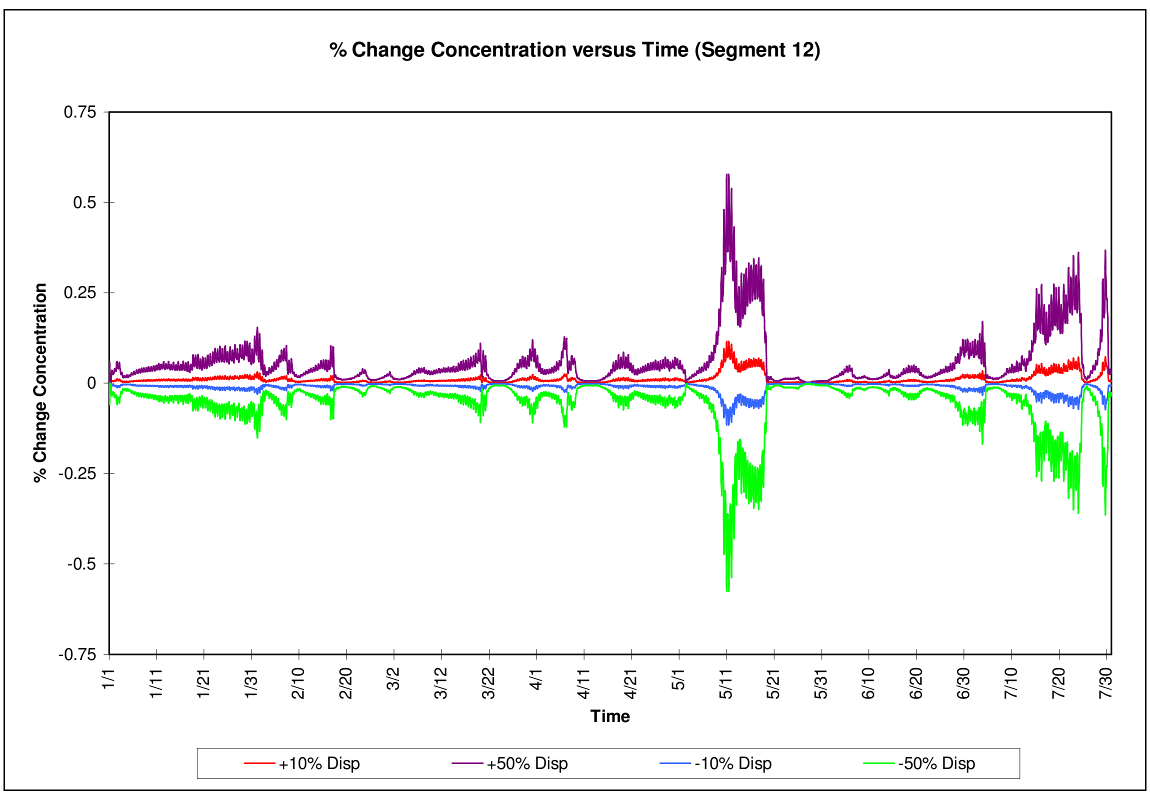

Figure 5.13b % Change Conc. versus % Change Dispersion Coeff. – Segment 12

Time-variable, fecal coliform boundary concentrations have the largest effect on WASP6.1 simulation results for the upstream portion (segment 12) of the Appomattox River. This is shown in Table 5.4 as well as Figure 5.10b above. The percent change in coliform concentration versus percent change in boundary concentrations remains approximately constant throughout the entire simulation period for the upstream portion of the model network. However, segment dispersion coefficients have the smallest impact on modeled fecal coliform concentrations both downstream and upstream. This is reflected in Tables 5.3 and 5.4 as well as Figures 5.13a and 5.13b. As a result, advective transport processes dominate coliform bacteria movement within the WASP6.1 water-quality model for this research. This phenomenon may be attributed to the physical geometry (long, narrow, and relatively shallow) of the tidal Appomattox River. Since the Appomattox River is fairly narrow and shallow, as compared to most tidal estuaries, the dispersive mixing cross-sectional areas (between segments) are relatively small. As a result, contaminant transport due to dispersion is limited.

The results obtained during model sensitivity analysis were used to optimize WASP6.1 input parameters during model calibration process. Sensitivity analysis proved to be quite effective in lending insight to which model parameters to modify for more reasonable model results.

5.2.2 Model Calibration

The time period selected for water-quality model calibration was October 1, 1998 through July 31, 2003. The selection of this simulation time period for model calibration is discussed in chapter 4. In addition, the calibration time period is the time period employed by MapTech, Inc. for HSPF water-quality calibration. The process utilized for input file generation remains the same as sensitivity analysis input file generation, which is discussed in chapter 4.

The calibration of the lower Appomattox River water quality model involved the following steps. First, simulated fecal coliform concentrations versus time were output at WASP6.1 segment 1. Next, modeled fecal coliform concentrations versus time were compared against observed instantaneous fecal coliform concentrations (logged by VADEQ at sampling station 2APP001.53) versus time. Input parameters, such as coliform die-off rate and segment dispersion coefficients, were adjusted until the modeled coliform concentrations converged upon the observed coliform concentrations. Results obtained during WASP6.1 sensitivity analysis were used in order to determine which input parameters to modify for more reasonable WASP6.1 results.

Figures 5.14a and 5.14b below are a graphical representation of the final WASP6.1 calibration for this research. Due to extensive experience with HSPF water-quality calibration, MapTech, Inc. provided the support necessary to finalize WASP6.1 model calibration. Modeled coliform concentrations do not correspond exactly to the observed instantaneous coliform concentrations. This discrepancy may be attributed to the use of a geometric average fecal coliform concentration at the downstream model boundary (confluence of Appomattox and James Rivers) instead of observed instantaneous time-variable coliform concentrations. However, detailed long-term records of fecal coliform concentrations do not exist at the downstream model boundary. WASP6.1 calibration results are summarized in chapter 6.

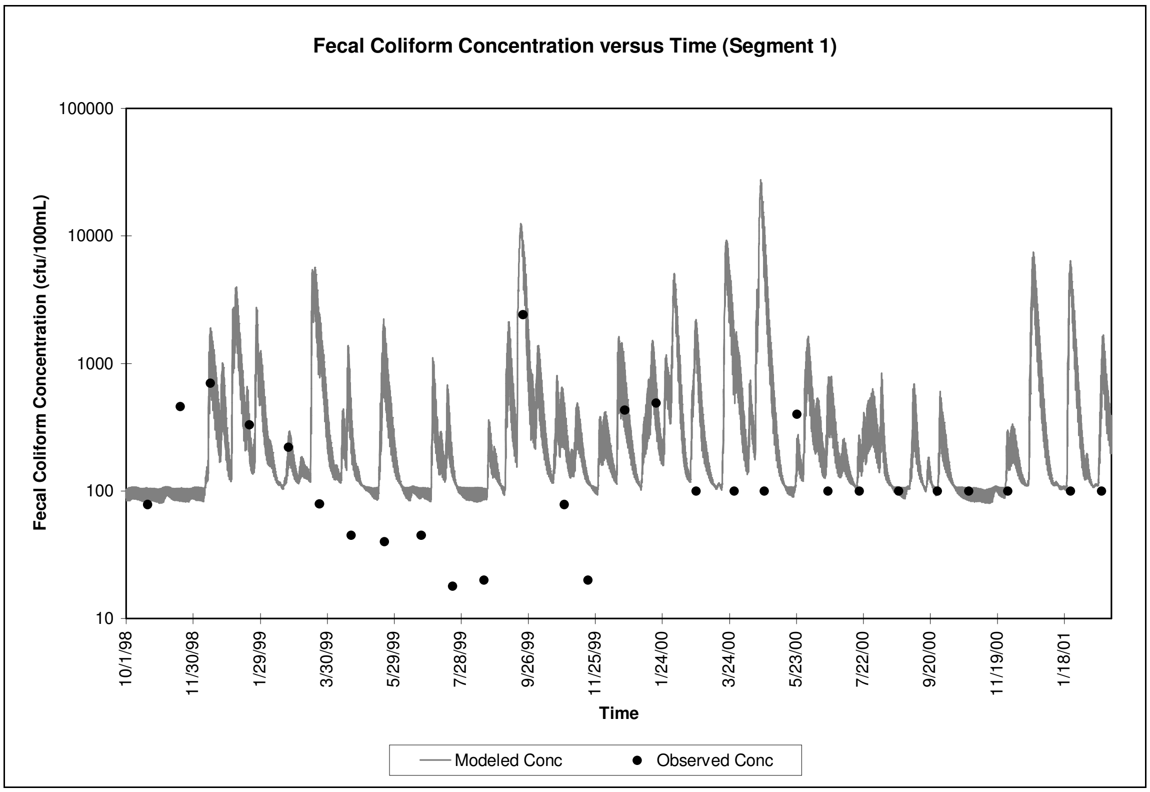

Figure 5.14a Modeled versus Observed Concentrations for WASP6.1 Calibration

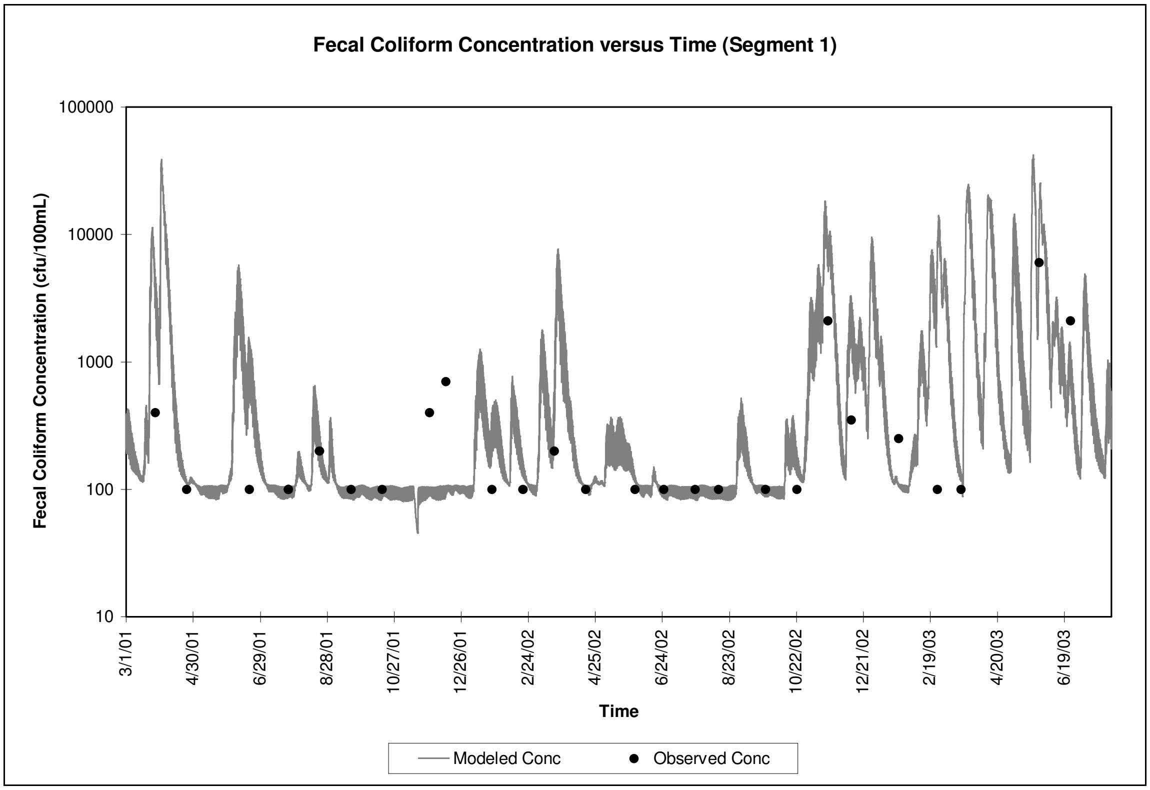

Figure 5.14b Modeled versus Observed Concentrations for WASP6.1 Calibration

Figure 5.15 below is a plot of modeled fecal coliform concentration versus observed fecal coliform concentration. After plotting the data, a linear regression was performed to determine a goodness-of-fit (r^2) value for WASP6.1 calibration. As stated earlier, as the r^2 value approaches 1.0, the modeled concentrations converge upon the observed concentrations, which is the ultimate goal of model calibration in this research.

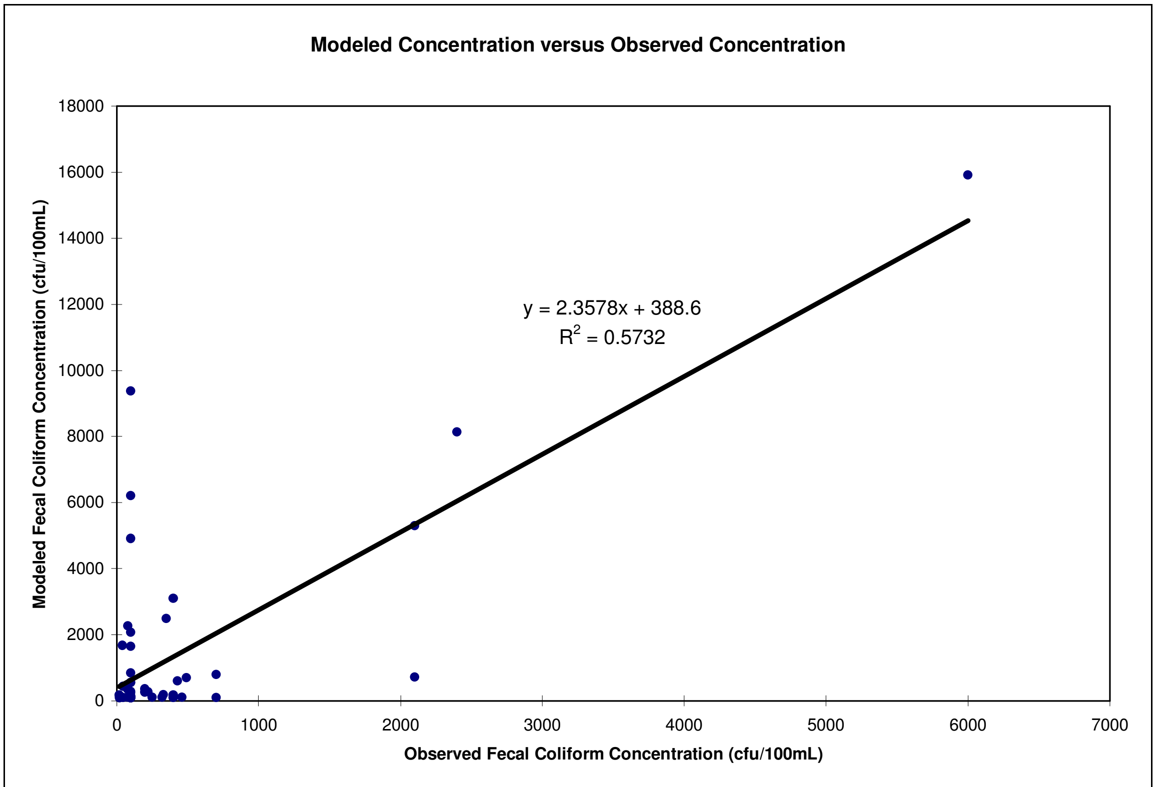

Figure 5.15 WASP6.1 Calibration Goodness-of-Fit (r^2) Value Determination

As shown in Figure 5.15, a goodness-of-fit (r^2) value of 0.573 was obtained for WASP6.1 calibration. As a result, modeled water concentrations are not directly equivalent to observed concentrations, which was noted earlier in Figures 5.14a and 5.14b.

5.2.3 Model Validation

The time period selected for WASP6.1 model validation was October 1, 1993 through September 30, 1998. The selection of this simulation time period is discussed in further detail in chapter 4. In addition, the validation time period is the time period employed by MapTech, Inc. for HSPF water quality validation. The process used for input file generation remains unchanged

In order to validate the lower Appomattox River water quality model, simulated fecal coliform concentrations versus time were output for WASP6.1 segment 1. The modeled coliform concentrations were then compared against observed instantaneous coliform concentrations to ensure the accuracy of model parameterization performed during calibration. Model input parameters remained unchanged throughout the validation process. This procedure is the same as that used during WASP6.1 calibration.

Figures 5.15a and 5.15b serve as a graphical representation of WASP6.1 parameter validation for the lower Appomattox River. As with model calibration, the modeled coliform concentrations do not correspond exactly to the observed instantaneous coliform concentrations. The primary cause of discrepancy is believed to be the use of a geometric average coliform concentration at the downstream model boundary instead of observed instantaneous coliform concentrations. WASP6.1 validation results are summarized in chapter 6.

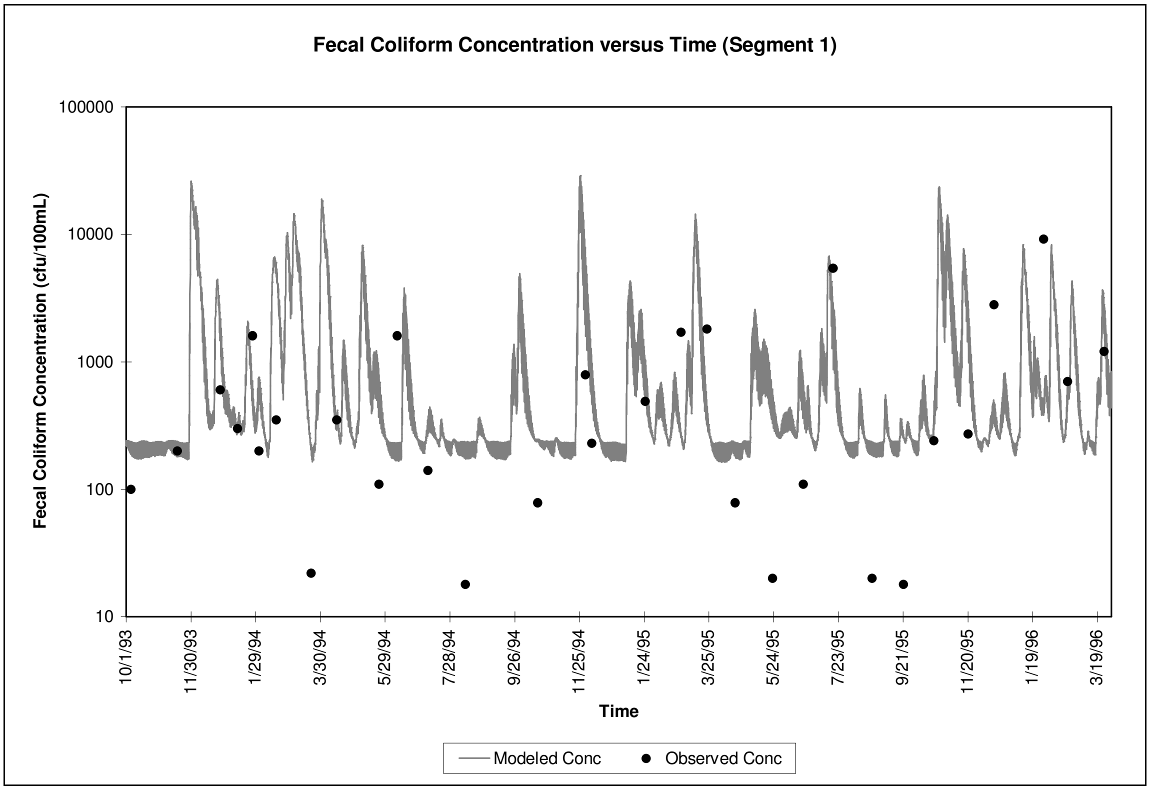

Figure 5.16a Modeled versus Observed Concentrations for WASP6.1 Validation

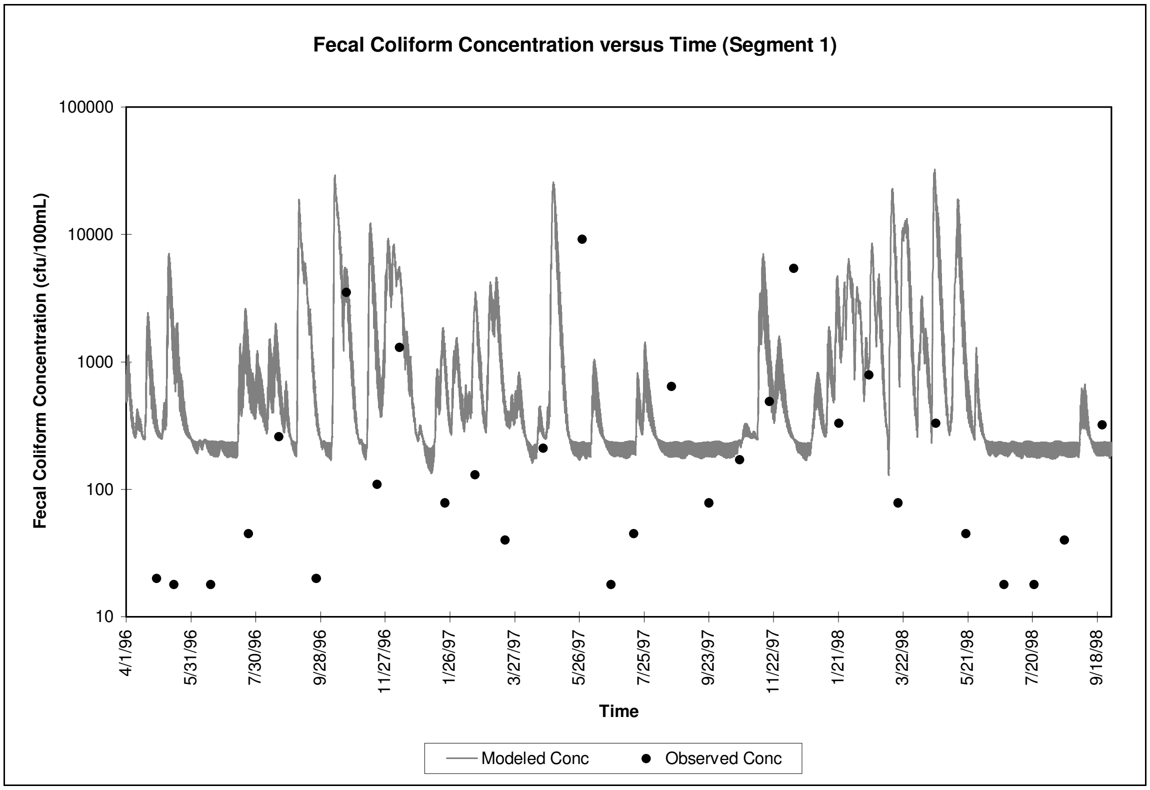

Figure 5.16b Modeled versus Observed Concentrations for WASP6.1 Validation

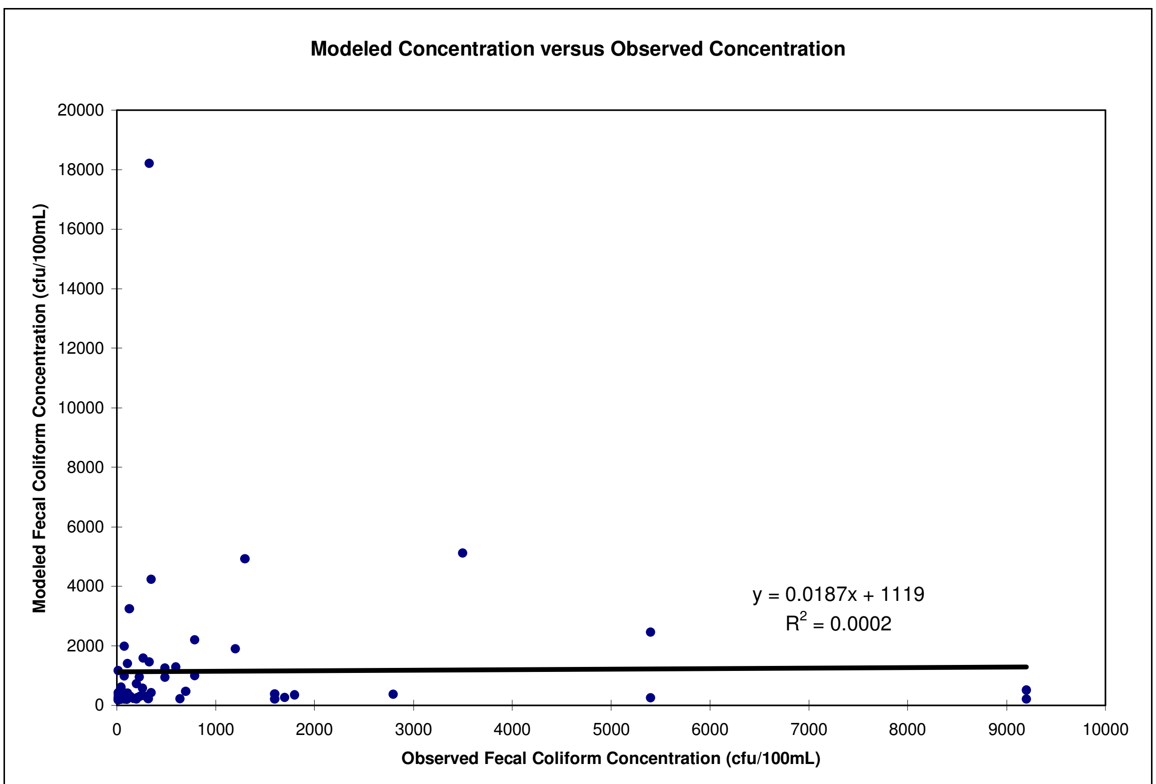

Figure 5.17 WASP6.1 Validation Goodness-of-Fit (r^2) Value Determination

Figure 5.17 above is a plot of modeled fecal coliform concentration versus observed fecal coliform concentration. After plotting the data, a goodness-of-fit (r^2) value of 0.829 was calculated and is shown in the above figure. Modeled concentrations are not directly equivalent to observed concentrations, which was noted earlier in Figures 5.16a and 5.16b.

5.2.4 Model Contingency Matrix Development

To further investigate the predictive capability of the WASP6.1 water quality model utilized in this application, the research team developed a single model contingency matrix, which encompasses both model calibration and validation. The contingency matrix is shown below in Table 5.5. It serves as a mechanism to compare the 118 (total number of water quality samples taken from October 1, 2003 through July 31, 2003) VADEQ observed instantaneous fecal coliform concentrations against their respective WASP6.1 predicted instantaneous concentrations. In addition, the matrix data is arranged into 2 categories, violations and non-violations. It should be noted that observed and modeled fecal coliform concentrations are considered to be water quality violations when their value equals or exceeds 400 cfu/100mL.

Table 5.5 WASP6.1 Model Contingency Matrix

		Observed Concentration	
		Violation	Non-violation
Modeled Concentration	Violation	19	31
	Non-violation	12	56

As shown in Table 5.5, the calibrated and validated water quality model accurately predicts the number of instantaneous water quality violations as well as non-violations approximately 63% of the time. As stated previously, the primary cause of discrepancy is believed to be the use of a geometric average fecal coliform concentration at the downstream seaward boundary for model calibration and validation.

6.0 Summary, Conclusions, and Future Directions

The development of a DYNHYD5 and WASP6.1 model for the lower Appomattox River has significantly advanced the process to examine water quality, as represented by fecal coliform within the waterbody. The models can be used to examine water quality scenarios that occur between October 1, 1993 and July 31, 2003. Specifically, the models could be utilized to perform TMDL studies on the lower Appomattox River. In addition, as more Appomattox River basin precipitation and streamflow data becomes publicly available, the model simulation period can be extended further towards the present day. The input parameters selected for the tidal Appomattox River produced reasonable results for DYNHYD5 and WASP6.1 sensitivity analysis, calibration, and validation. Modeled water surface elevations and fecal coliform concentrations were compared against their respective observed values to achieve model calibration and validation. Potential improvements could be made to both the DYNHYD5 and WASP6.1 inputs datasets and are discussed briefly below. However, a regimented sampling program would have to be established to make these improvements a reality.

6.1 Review of Objectives

This research was directed at the objectives detailed in chapter 1. The objectives are summarized in the list below:

- **Examine an array of candidate estuary hydrodynamic and water quality models.**
  A number of different hydrodynamic and water-quality models were reviewed for this research. Government agencies and institutions that provided information for this review include USEPA, USACE, Portland State University, and VIMS (College of William and Mary). Model attributes were summarized in 3 model selection matrices, Tables C.1, C.2, and C.3. The models reviewed are discussed in chapter 2.

- **Select and implement a hydrodynamic and water quality model utilizing existing datasets.**
  The research team selected DYNHYD5 coupled with WASP6.1 as the modeling software to be used for this research. The arguments supporting model selection are examined in chapter 2. DYNHYD5 and WASP6.1 models were implemented using data collected from USGS as well as numerous field visits. Model development is explained in detail in chapter 3.

- **Make use of streamflows and contaminant loadings from HSPF simulation runs as inputs to the hydrodynamic and water quality models.**
  HSPF streamflow outputs were successfully exported and then reformatted for implementation into the necessary DYNHYD5 input files. Contaminant loadings from HSPF were also successfully exported and imported into WASP6.1. The procedures used to generate DYNHYD5 and WASP6.1 input files are documented in chapter 4.

- **Compare the results of the hydrodynamic and water quality models to previously observed values for predetermined calibration and validation time periods.**
  DYNHYD5 and WASP6.1 sensitivity to specific model parameters were determined with a series of model runs. These results of the sensitivity analysis are presented in chapter 5. Utilizing existing data during a predetermined calibration period, DYNHYD5 model parameters were optimized. To verify these refined DYNHYD5 model parameters, the model was executed for a validation period different from the calibration time frame. After successful calibration and validation of DYNHYD5, this optimization procedure was repeated for WASP6.1. Model calibration and validation results are presented in chapter 5.

- **Investigate the possible use of other models in order to estimate estuary hydrodynamics and water quality as well as determine their required inputs and solution techniques.**
  Hydrodynamic and water quality simulation in the lower Appomattox can potentially be improved through the use of EFDC. The EFDC model is briefly discussed in chapter 2. A more detailed investigation of the modeling software was performed. This investigation presents the steps necessary and input data required to successful implement the EFDC software on the lower Appomattox River. The results are presented at the end of this chapter.

6.2 Summary of DYNHYD5 Model Results

DYNHYD5 showed significant sensitivity to boundary tidal heights (seaward boundary conditions) in the downstream portion of the lower Appomattox River. The model did not show significant sensitivity to overland flow, instream flow, or Manning's roughness coefficients in the downstream direction. As a result, the boundary tidal heights govern the modeled water surface elevations in downstream portion of the Appomattox River. For the upstream portion of the model network, DYNHYD5 also showed significant sensitivity to boundary tidal heights. In addition, the model showed sensitivity to instream flow and Manning's roughness coefficients. Overland flow did not have a significant impact on model results in the upstream direction. Therefore, upstream model results were governed by the combination of tidal heights, instream flow, and Manning's roughness coefficients.

May 22, 2003 through June 13, 2003 was chosen as the simulation time period for hydrodynamic calibration. Modeled water surface elevations were compared with observed water surface elevations and reasonable results were obtained. In addition, a goodness-of-fit value of 0.749 was calculated using linear regression analysis. June 14, 2003 through July 5, 2003 was selected as the simulation time period for input parameter validation. Reasonable results were obtained and a goodness-of-fit value of 0.829 was calculated. Also, a goodness-of-fit value of 0.788 was determined for the entire simulation time period. As a result, DYNHYD5 proved to be an effective tool for reproducing hydrodynamic conditions within the lower Appomattox River.

6.3 Summary of WASP6.1 Model Results

WASP6.1 showed significant sensitivity to boundary coliform concentrations, segment coliform loading rates, and coliform die-off in the downstream and upstream portions of the model network. The model did not show significant sensitivity to segment dispersion coefficients. As a result, advective transport dominates coliform bacteria movement within the lower Appomattox River. In addition, the combination of boundary concentrations, loading rates, and coliform die-off governs water quality results.

October 1, 1998 through July 31, 2003 was selected as the simulation time period for water quality calibration. Modeled fecal coliform concentrations were compared with observed instantaneous fecal coliform concentrations and reasonable results were obtained. October 1, 1993 through September 30, 1998 was chosen as the simulation time period for input parameter verification. Input parameters selected during model calibration produced moderate results. As a result, WASP6.1 proved to be a capable tool for simulating the fate and transport of fecal coliform bacteria within the lower Appomattox River.

6.4 Evaluation of DYNHYD5 and WASP6.1 Model Architecture in this Application

The DYNHYD5 hydrodynamic model proved to extremely sensitive both upstream and downstream to the tidal heights specified at the downstream seaward boundary. One deficiency encountered in estuary modeling is the lack of observed data (i.e. water surface elevations and water velocities) to be used for hydrodynamic model set up, calibration, and validation. Due to a lack of observed data, NOAA tide predictions were used for tidal heights at the downstream seaward boundary. However, tide predictions are educated estimates of water surface elevation and may not truly or accurately represent the system being modeled. DYNHYD5 was found to under predict as well as over predict water surface elevations at the model calibration and validation location (DYNHYD5 junction 2). This implies that the specified tidal height values need further refinement in order to achieve a more accurate model calibration and validation.

WASP6.1 was found to be sensitive to boundary concentration, loading rate, and coliform die-off rate in the downstream water quality model network. For this research, upstream boundary concentrations and coliform loading rates were determined with HSPF and remained unchanged for use with WASP6.1. As noted above, one weakness encountered in estuary modeling is the lack of observed data. Due to a lack of long-term, detailed observed data, an average coliform concentration was used for the downstream boundary (confluence of Appomattox and James Rivers) concentration instead of time-variable coliform concentrations. After refining the coliform die-off rate, WASP6.1 was found to over predict as well as under predict fecal coliform concentrations at the model calibration and validation location (WASP6.1 segment 1). This indicates that the downstream average coliform concentration needs refinement, specifically time-variable coliform concentrations should be utilized.

Overall, DYNHYD5 produced reasonable results for the hydrodynamic simulation of the lower Appomattox River, Virginia. In addition, WASP6.1 demonstrated reasonable accuracy for the water quality simulation of fecal coliforms within the lower Appomattox River. Potential refinements to both models could improve model calibration and validation results. These refinements are predominately dependent upon the collection of long-term records of water surface elevation and fecal coliform concentrations at specific model calibration locations. However, detailed data collection is time consuming as well as extremely costly under most circumstances. Due to the time constraints placed on this research as well as the lack of detailed long-term observed data sets, the DYNHYD5 and WASP6.1 model architecture proved to be very effective and efficient in the hydrodynamic and water quality simulation of fecal coliforms within the lower Appomattox River.

6.5 DYNHYD5 and WASP6.1 Model Limitations in this Application

The predictive capability of the hydrodynamic and water quality models utilized was limited by the data available for model set up, parameter calibration and validation. Model application limitations are summarized in the list below:

- **DYNHYD5 should be utilized to estimate estuary water surface elevations and junction volumes.**
  Due to a lack of velocity measurements, modeled water velocities could not be verified against observed data.

- **WASP6.1 should be employed to predict estuary fecal coliform concentrations assuming water temperature remains constant at 20ºC.**
  Due to a lack of observed data, temperature effects on fecal coliform die-off were not taken into consideration in this research.

- **WASP6.1 should be utilized to estimate estuary fecal coliform concentrations in circumstances where downstream boundary concentrations can be approximated by a geometric average boundary concentration.**
  A regular time-series of fecal coliform concentration at the downstream model boundary does not exist for use in this research. Therefore, a geometric average boundary concentration was established for each modeling period.

- **WASP6.1 should be employed to predict fecal coliform concentrations assuming estuary physical, chemical, and biological processes can be represented by first-order reaction kinetics.**
  The WASP6.1 model developed for use in this research does not include a fecal coliform routine that fully accounts for salinity concentration, attachment to sediment, or temperature effects on fecal coliform die-off. Instead, these processes were represented by first-order reaction kinetics. While this may be considered adequate in simple linear systems, it cannot account for dynamic changes in fecal coliform concentrations in more complex systems.

6.6 Future Directions in Estuary Modeling

Current computer-based hydrodynamic models allow the engineer or hydrologist to perform simulations in 3 dimensions. Modelers have the capability of simulating in-stream velocities in the longitudinal, lateral, and vertical directions. If necessary, one can predict velocities associated with flow moving the length of the river, velocities associated with flow moving from the center of the river to the banks or vice versa, and velocities associated with flow moving from the river bed to the water surface or vice versa. The same principles apply to current computer-based water quality models. Modelers have the tools necessary to simulate changing pollutant concentrations in 3 dimensions.

A major consideration during model implementation is whether to develop a 3-dimensional model if a 2-dimensional or 1-dimensional model will provide similar results. This consideration is partially due to the fact that the data requirements for a 3-dimensional model are highly extensive. In addition, the time and money required to set up, calibrate, and validate a 3-dimensional model are typically greater than those necessary for 2- and 1-dimensional models, especially if no data is present at the onset of model implementation. As a result, future research should examine the potential development of a parameter or series of parameters to be calculated before model implementation in order to determine the model dimensionality required for accurate estuary simulation.

With respect to the lower Appomattox River, future research should explore the possible development and implementation of a 2- or 3-dimensional hydrodynamic and water quality model within the river system. As previously noted, WASP6.1 can be utilized for 2- or 3-dimensional water quality simulation. However, a new hydrodynamic model must be coupled with WASP6.1. One proposed hydrodynamic model is the Environmental Fluid Dynamics Code (EFDC), which was developed at the Virginia Institute of Marine Science (VIMS). As shown in Tables C.1 and C.2 in Appendix C, theses model has been utilized in numerous water quality studies with extensive use in tidal estuaries. Therefore, WASP6.1 coupled with EFDC is a good candidate model for 2- and 3-dimensional hydrodynamic and water quality simulation within the lower Appomattox River.

6.6.1 Development of Parameters for Model Dimensionality Selection

Presently, hydrodynamic and water quality model dimensionality is chosen on an as needed basis. For example, modelers would most likely select a 2-dimensional, laterally averaged model to perform simulations of reservoir stratification. In addition, a 2-dimensional vertically averaged model would most likely be employed to perform simulations within a long, wide, and relatively shallow estuary. However, maybe a 3-dimensional model should be utilized to perform reservoir stratification simulations or a 1-dimensional model could provide exactly the same results as the 2-dimensional model for the estuary. As a result, a list of parameters could be researched and established to aid in the selection of an appropriate model with appropriate dimensional capability.

Utilizing the existing bathymetry data located on USGS 7.5-minute quadrangles, one can approximate the average width and depth at various locations along the waterbody in question. These parameters could provide an initial estimate of the required model dimensionality needed to accurately represent the system. Observed channel velocities in the longitudinal, lateral, and vertical directions could then be employed to further refine the selection of an appropriate model with appropriate dimensional capability. Finally, a survey of observed or collected data could be used to determine if the existing data permits the use of the previously selected model dimensionality. The aforementioned parameters could be established for previous as well as new modeling studies and then summarized in matrix form. The matrix could then be used to aid in the informed selection of a dimensionally appropriate model for a given reservoir, river, or estuary.

The ultimate goal of guidelines for model dimensionality would be the development of a single parameter to be calculated before model selection and implementation. The parameter should be readily obtained from existing or newly collected data sets and could be likened to the well-known parameter for flow regime determination, Reynolds' Number. A specific range of values would be used to determine if the model needed to be implemented in 1, 2, or 3 dimensions to accurately represent the system at hand. To establish a relationship between parameter inputs and required model dimensionality, a significant amount of modeling research would have to be performed in 1, 2, and 3, dimensions. Hydrodynamic and water quality models would have to be implemented on a number of different estuaries with varying physical geometry. This research is currently beyond the capabilities of DYHHYD5 since it only performs hydrodynamic simulations in the longitudinal direction. However, WASP6.1 is capable of performing simulations in 3 dimensions and could be coupled with a 3-dimensional hydrodynamic model such as EFDC to complete the required research.

6.6.2 Two-Dimensional Modeling of Lower Appomattox River, VA

The lower Appomattox River is a relatively long, narrow, and shallow waterbody when compared against most other tidally influenced estuaries (i.e. Chesapeake Bay, James River, Rappahannock River, York River, and Potomac River). As a result, a 1-dimensional hydrodynamic and water quality was selected and then implemented to simulate the fate and transport of fecal coliforms within the river system. As noted in chapter 2, significant advances in computer-based modeling now enable engineers, hydrologists, and modelers to perform hydrodynamic and water quality simulations in 1, 2, and 3 dimensions. Therefore, the next logical step concerning the lower Appomattox River would be to develop and implement a 2-dimensional hydrodynamic and water quality model. The 2-dimensional model and/or models could be utilized for comparison purposes as well as initiate the research regarding parameter development for model dimensionality selection noted in the previous section.

As noted in chapter 2, the Environmental Fluid Dynamics Code (EFDC) is capable of hydrodynamic modeling in 3 dimensions and is fully compatible with WASP6.1. Therefore, the remaining portions of this section will discuss the EFDC model inputs and

WASP6.1 changes that will be required to simulate in 2 dimensions. Due to the relatively shallow nature of the lower Appomattox River, a 2-dimensional vertically averaged model will be considered initially.

6.6.2.1 Two-Dimensional Hydrodynamic Modeling using EFDC (Hamrick ,1996)

Dr. John Hamrick developed EFDC at the Virginia Institute of Marine Science, and a streamlined version of the model (EFDC-HYDRO) can be obtained from USEPA's Watershed and Water Quality Modeling Technical Support Center located in Athens, Georgia. The current model software is fully compatible with WASP6.1 and can be employed for simulations in 1, 2, or 3 dimensions. Two-dimensional vertically averaged model inputs are discussed below.

<u>Waterbody Geometry Data:</u>

Unlike DYNHYD5, EFDC utilizes a grid of quadrilateral and triangular cells to approximate the horizontal geometry of the system to be modeled. The physical properties of each cell are contained within a single ASCII-formatted text file (dxdy.inp). Cell physical properties include: length (dx), width (dy), initial water depth, bottom bed elevation, roughness height, and vegetation type. A second text file (lxly.inp) is used to specify the coordinates of cell centers as well as rotation matrix components if necessary. In addition, the lxly.inp text file is only utilized during graphics output. The two aforementioned text files are generated with the aid of the EFDC preprocessor, GEFDC.

In order to utilize GEFDC, 7 ASCII-formatted input files must be created beforehand. The first input file (cell.inp) contains a grid of cell identifiers, numbers 1 through 9 defining the type of cell in the corresponding grid location. The second input file (depdat.inp) consists of varying water depth or bathymetry data. The third input file (gcell.inp) is utilized to convert curvilinear grid graphics to Cartesian grid rectangular. The fourth file (gridext.inp) is comprised of the coordinates for each corner of a "wet" cell. Vegetation type classes are specified in the file vege.inp. In addition, varying bottom roughness is contained within the file zrough.inp. The seventh input file (gefdc.inp) is the master input file for the preprocessor. These 7 input files are used in conjunction with GEFDC to create the model grid as well as define the properties of each cell within the grid.

Estuary geometry input file generation for EFDC is inherently more complicated than the procedure used in DYNHYD5. This is due to the fact that EFDC uses a grid of cells to represent waterbody geometry and not a series of channels and junctions. In addition, EFDC makes use of 7 different input files in order to generate the model grid as well as define the properties of each cell within the grid, whereas all DYNHYD5 data is contained within a single text file. A majority of the channel and junction data collected on the lower Appomattox River could be reused to develop the necessary preprocessor input files to be used for grid and grid cell parameter generation. Since the 2-dimensional model being considered is vertically averaged, only 1 layer will exist in the vertical direction. In addition, a minimum of 2 cells will be established in the lateral direction.

As a result, flow will now be permitted to move from channel center to channel banks and vice versa as well as along the main channel axis (longitudinal direction).

Inflow Data:

Constant or time-variable inflow data for model layers is contained within a separate ASCII-formatted input file (qser.inp). Inflow parameters include: time series format identifier, number of inflow data points, conversion factor for changing inflow time units to seconds, additive time adjustment if required, multiplying conversion factor if required, additive conversion if required, and layer weighting factors if utilized. The previously established constant and time-variable DYNHYD5 inflows could be easily adapted for use within the EFDC modeling software.

Atmospheric, Wind, Precipitation, and Evaporation Data:

Time-variable atmospheric and wind forces as well as precipitation and evaporation data are specified within a single and separate text file (aser.inp). Initial input parameters include: number of time data points, time units conversion factor, additive time constant, wind speed conversion factor, rainfall rate conversion factor, and evaporation rate conversion factor. Additional parameters include time, wind speed, wind direction, wet and dry bulb temperature, rainfall rate, and evaporation rate. Rainfall and evaporation rates have been taken into account during HSPF simulation runs. In addition, due to a lack of detailed observed data, wind forcing was not taken into account within DYNHYD5. As a result, these parameters would not have to be specified within EFDC to perform initial 2-dimensional vertically averaged simulations.

Open Boundary Data:

The text file pser.inp contains time-variable water surface elevations for open (i.e. seaward) boundaries. Input file parameters include the number of time data points, time units conversion factor, water surface elevation conversion factor, time of occurrence, and time-variable water surface elevations. The NOAA tide predictions formatted for use with DYNHYD5 can be readily reformatted for use with EFDC, therefore providing an easy transition between the 2 modeling programs.

Linkage to WASP Modeling Software:

EFDC simulated hydrodynamics can easily be linked to the WASP model software with the aid of a separate text file (efdc.wsp). Within the input file, users must specify whether to create an ASCII-formatted external hydrodynamics file or a binary-formatted external hydrodynamics file. Either format is supported by the current version of WASP model software, WASP6.1. Within the external hydrodynamics file, EFDC will write time-variable cell volumes, instream flow linkages, and cell diffusion/dispersion linkages.

Simulation Control Data:

A majority of the required EFDC input data is contained within separate input text files as noted above. However, model input parameters detailing simulation control, output control, and model domain are contained within the master input file, efdc.inp. The master input file is arranged into a series of 62 card images, which contain information pertaining to simulation time step, printout time step, model grid dimensions, layer thickness, volumetric inflow locations, open boundary locations, WASP linkage options, and an ongoing list of other model parameters. Readers are urged to review chapter 4 of the EFDC user's manual (Hamrick, 1996) for a detailed discussion of the master input file. DYNHYD5 simulation control and output parameters can be readily transferred over for use within the EFDC software.

Model Equations and Solution Techniques:

As stated by Hamrick (1996), the EFDC model solves the three-dimensional, vertically hydrostatic, free surface, turbulent averaged equations of motion for a variable density fluid. Therefore, the 3-dimensional continuity equation (2.15) presented in chapter 2 remains unchanged for use within EFDC. However, slight modifications have been made to the 3-dimensional equations of momentum (2.16, 2.17, and 2.18) and for brevity will not be presented here. For a complete discussion on EFDC model theory see "A Three-Dimensional Environmental Fluid Dynamics Computer Code: Theoretical and Computational Aspects" prepared by Hamrick (1992).

To perform computations, EFDC utilizes a spatial finite difference solution technique. Time integration is achieved with the aid of an internal-external mode, finite difference scheme. The internal solution technique is implicit with regards to vertical diffusion, whereas the external solution technique is semi-implicit. Hamrick (1992) discusses EFDC computational aspects more thoroughly in the aforementioned reference.

A majority of the data collected for use with DYNHYD5 can be readily adapted for use with EFDC. As a result, a fairly simple 2-dimensional hydrodynamic model could be developed for the lower Appomattox River. However, this would require more bathymetry data to be collected. Given the time to examine all aspects of EFDC (preprocessor and postprocessor included), the researchers believe a detailed 2-dimensional hydrodynamic model of the lower Appomattox River could be developed.

6.6.2.2 Two-Dimensional Water Quality Modeling Using WASP6.1

As noted in chapter 2, WASP6.1 can be used to perform water quality simulations in 1, 2, and 3 dimensions. In addition, the current model software can be linked to EFDC through the use of an EFDC generated external hydrodynamics file. A majority of the water quality data collected for use with DYNHYD5/WASP6.1 (i.e. boundary concentrations and coliform loading rates) can be reused for EFDC/WASP6.1 water quality simulations. Cell volumes, velocities, instream flow linkages and diffusion/dispersion linkages are contained within the external hydrodynamics file. Therefore, WASP6.1 set up would be simplified because dispersive exchange functions are predefined within the external linkage file. In addition, the remaining model input parameters could be adapted from previous DYNHYD5/WASP6.1 water quality simulation runs. As a result, a 2-dimensional water quality model of the lower Appomattox River could be readily developed from existing datasets and a new EFDC hydrodynamics linkage file.

6.7 Research Conclusions

A number of different factors dictated the selection and utilization of a 1-dimensional hydrodynamic and water quality model for this research. The lower Appomattox River is relatively long, narrow, and shallow when compared against other tidally influenced estuaries within the state of Virginia (i.e. Chesapeake Bay, James River, Rappahannock River, and York River). As a result of the physical geometry present, a 1-dimensional hydrodynamic and water quality model was suggested for use within the lower Appomattox River. In addition, a lack of detailed bottom topography or bathymetry data within the area of interest hindered the development of a 2- or 3-dimensional model for this research. Computer-based models can require a significant amount of time for set up, calibration, and validation, especially when the model user has not previously utilized them. The amount of time required to set up, calibrate, and validate a 1-dimensional hydrodynamic and water quality model is significantly less than that required for an equivalent 2-, or 3-dimensional model. Due to time constraints placed on this research as well as the aforementioned arguments, a 1-dimensional hydrodynamic and water quality model was chosen for simulation purposes.

After performing a detailed literature review, the research team selected DYNHYD5 coupled with WASP6.1 as the model architecture for this research. Detailed arguments for their selection are presented in chapter 2. In summary, DYNHYD5 and WASP6.1 are well matched computationally to the needs of this research and to the physical characteristics of the lower Appomattox River system. Data input requirements, particularly channel bathymetry, also are compatible with the data currently available to this research. WASP6.1 and DYHHYD5 were both developed by USEPA and have been used extensively in order to perform USEPA water quality studies for tidal estuaries. In addition, extensive model documentation is readily available from the USEPA website. As a result, model availability and user support is not a critical issue.

With the data available and time constraints present, reasonable results were obtained for hydrodynamic and water quality model calibration and validation. Therefore, DYNHYD5 coupled with WASP6.1 proved to be quite effective in the hydrodynamic and water quality simulation of fecal coliforms within the lower Appomattox River. As a result, the secondary objective of this research was achieved, which was to investigate the use of multiple models to estimate estuary hydrodynamics and water quality. In addition, armed with the hydrodynamic and water quality background presented in chapters 2 and 3 as well as with the newly developed DYNHYD5 and WASP6.1 models, engineers and hydrologists can now investigate proposals for improving water quality within the lower Appomattox River. Therefore, advancing the analytical process by which various proposals for improving water within the lower Appomattox River could be examined and ultimately satisfying the primary objective of this research.