

Stage and Water Quality Compartmental Model of an Everglades Wetland

Hamid Bazgirkhoob

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The Center for Louisiana Inland Water Studies, University of Louisiana –
Lafayette

Ehab A. Meselhe – Director and Principle Investigator

The Arthur R. Marshall Loxahatchee National Wildlife Refuge, US Fish and
Wildlife Service

Michael G. Waldon, Technical Cooperator

ABSTRACT : Cluster analysis was applied to objectively determine the number of compartments and to spatially delineate compartments with similar features in the Arthur R. Marshall Loxahatchee National Wildlife Refuge which led to delineate the 9-Compartment Model structure based on the analysis of concentrations of chloride, total phosphorus, sulfate, and calcium. The 39-Compartment Model was built by analyzing the water quality gradient from the calibration and validation of the 9-Compartment Model, and professional judgment by analyzing information such as the vegetation/elevation map of the Refuge.

The 39-Compartment Model results represent spatially aggregated canal and marsh values for all state variables (e.g., volume, stage, and water quality parameters). The 39-Compartment Model predicts water stage very well for canal and marsh. The model also predicts the concentration of three constituents (Cl, SO₄, and TP) reasonably well. It is evinced that in the Refuge, the inflow structures in the north have strong impact to the flows in the canal and the northern marsh. Automated calibration of the seepage coefficients for the marsh and the canal revealed that the seepage loss in canals for the 39-Compartment Model is larger than that for the 9-Compartment Model.

The 39-Compartment Model and the Spatially Explicit Model (Mike Flood) were quantitatively evaluated vs. observed data. Although, the 39-Compartment Model can be used to detect water quality variations along western and eastern gradients as well as north-to-south gradient, due to its spatially aggregated nature, the model was not designed to be used to analyze site specific events. But, the Spatially Explicit Model (Mike Flood) can provide more accurate prediction of the observed data for the Refuge. The Spatially Explicit Model results provide detailed spatial and temporal information of hydrodynamic and water quality state variables. This model can be used to analyze site specific events. Depending on the time scale of input data, Mike Flood can be used for analyzing short term (transient) to long term (daily, monthly or annual) events. In view of its computational cost, it is feasible to run decadal simulation within reasonable amount of time.

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Hamid Bazgirkhoob

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Hamid Bazgirkhoob

APPROVED:

Ehab Meselhe, Co-chair
Professor of Civil Engineering

Chunfang Chen, Co-chair
Assistant Professor of Civil Engineering

Emad Habib
Associate Professor of Civil Engineering

Daniel Dianchen Gang
Associate Professor of Civil Engineering

Michael G. Waldon
U.S. Fish and Wildlife Service
Arthur R. Marshall Loxahatchee National
Wildlife Refuge

David Breaux
Dean of the Graduate School

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1 Introduction

Everglades wetlands may be changed to a focal point for advancing the hydrological, ecological, and environmental sciences as a result of restoration efforts. In general, the ability to predict the effects of manipulation of water operations is a chief factor in the success of wetland management and restoration (Gilvear and Bradley, 2000; Hollis and Thompson, 1998). In specific, many studies have been aimed at modeling hydrologic processes and the fate and transport of nutrients. As a result of these studies, models have been developed and modified to simulate certain physical, hydrologic, or water quality alterations. These models can be calibrated and validated with observed data for different time periods. A calibrated hydrodynamic and water quality model provides managers and planners with information on movement of water, and the fate and transport of constituents (Kadlec and Hammer, 1988; Tsanis et al., 1998; Koskiahio, 2003). Modeling also provides further analysis of observed data by indicating the weaknesses of sample timing and spatial resolution (Roth, 2009). Models can also be applied for water management schedules, and testing scenarios.

Wang et al. (2008) applied cluster analysis to objectively determine the number of compartments for modeling the Refuge. Cluster Analysis led to the design of a 9-compartment model structure based on the analysis of concentrations of chloride, total phosphorus, sulfate, and calcium measured at sites distributed throughout the Refuge for the period of 1995–2006. The 9-Compartment Model was implemented in Berkeley Madonna which is an ordinary differential equation solver. The 9-Compartment Model consists of 3 canal and 6 marsh compartments as shown in Fig. 8. Although being an improvement over

the 4-Compartment Model, the 9-Compartment Model still has limitation in analyzing site specific events.

By analysis of the water quality gradient from the calibration and validation of the 9-Compartment Model, and the judgment based on the information such as vegetation/bathymetry map of the Refuge, a 39-Compartment Model was built in Berkeley Madonna (Wang, unpublished). This delineation led to the division of the 9 compartments into 39 compartments with 11 canal and 28 marsh compartments. This model supports investigation of the spatial details of the water and constituent movement in the Refuge. Berkeley Madonna allows users to implement models in either a graphical, object-based environment or an equation editing window. Additionally, the flexibility of the Madonna environment allows multiple kinetic formulations for constituent fate and transport, and scenarios analysis. Such applications would not have been convenient or possible with the previous setup of the SRSM (Roth, 2009). The objective of this thesis is to a) document the 39-Compartment Model calibration and validation, and b) continue the work of model comparison.

1.1 Background

The Arthur R. Marshall Loxahatchee National Wildlife Refuge overlays a 58,725 ha, remnant of the Northern Everglades located in Palm Beach County, Florida (USFWS, 2000) which is termed Water Conservation Area 1 (WCA-1) (Fig. 1). The Refuge is managed by the United States Fish and Wildlife Service (USFWS). The USFWS recognized that there have been changes to the Refuge's water quantity, timing, and quality which have caused

negative impacts to the Refuge's ecosystem. The Refuge is impacted by changes in water flow and stage (Brandt et al., 2000; USFWS, 2000; Brandt, 2006), excessive nutrient loading (Newman et al., 1997; USFWS, 2000), and altered dissolved mineral concentrations including chloride (Swift, 1981; Swift, 1984; Swift and Nicholas, 1987; Browder et al., 1991; Browder et al., 1994; McCormick and Crawford, 2006). The Refuge has supported development of hydrodynamic and water quality models to gain a better understanding of these impacts, and to evaluate alternative management options that may reduce these impacts.

1.2 Site Description

The Refuge is located 11.3 km west of the city of Boynton Beach, Florida in the southeastern United States (Fig. 1). It is enclosed within a levee system and a borrow canal along the interior of the levee (Richardson et al., 1990). The Refuge landscape consists of a complex mosaic of wetland communities including sloughs, wet prairies, sawgrass, brush, and finally tree islands occurring at the dryer end of the scale (USFWS, 2000). Refuge water conditions are controlled by the inflows and outflows through pumps and gates along the rim canal. Land use in areas bordering the Refuge varies from drained agricultural land (the Everglades Agricultural Area) on the northwest boundary, urban development to the east, and Everglades wetlands of Water Conservation Area 2A (WCA-2A) located southwest of the Refuge.

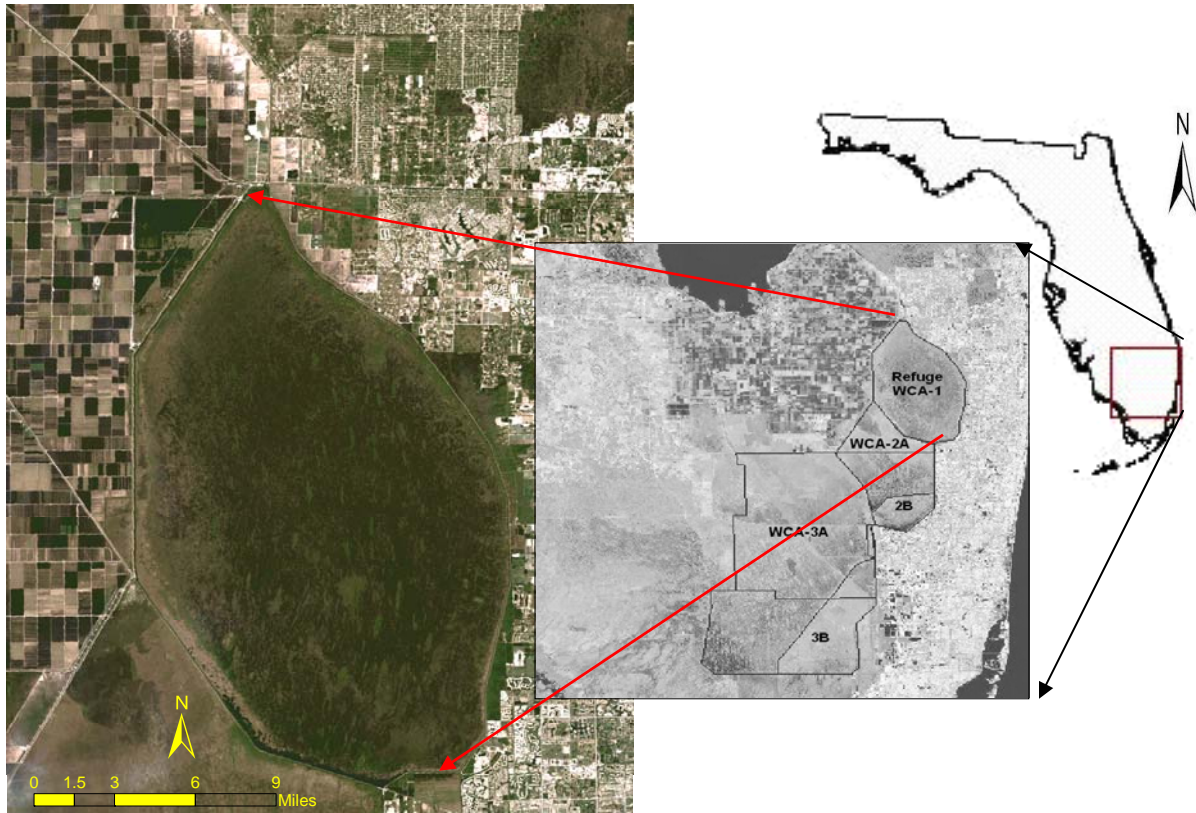


Figure 1 – Satellite image and location of the Arthur R. Marshall Loxahatchee National Wildlife Refuge within the State of Florida. (Adapted from SFWMD (2000a))

Refuge topography is characterized by a fairly flat interior marsh elevation (roughly 560 km² area) and a varying-section rim canal (approximately 100 km in length). The marsh elevation data were available from the United State Geological Survey (USGS) on a 400 by 400 m grid (Desmond, 2003) (m represents meter in this document). The elevation ranges from 5.64 to 3.23 m (NGVD29) decreasing slightly from north to south, which at times, may direct a slow southward surface water flow (Meselhe et al., 2005) (Fig. 2).

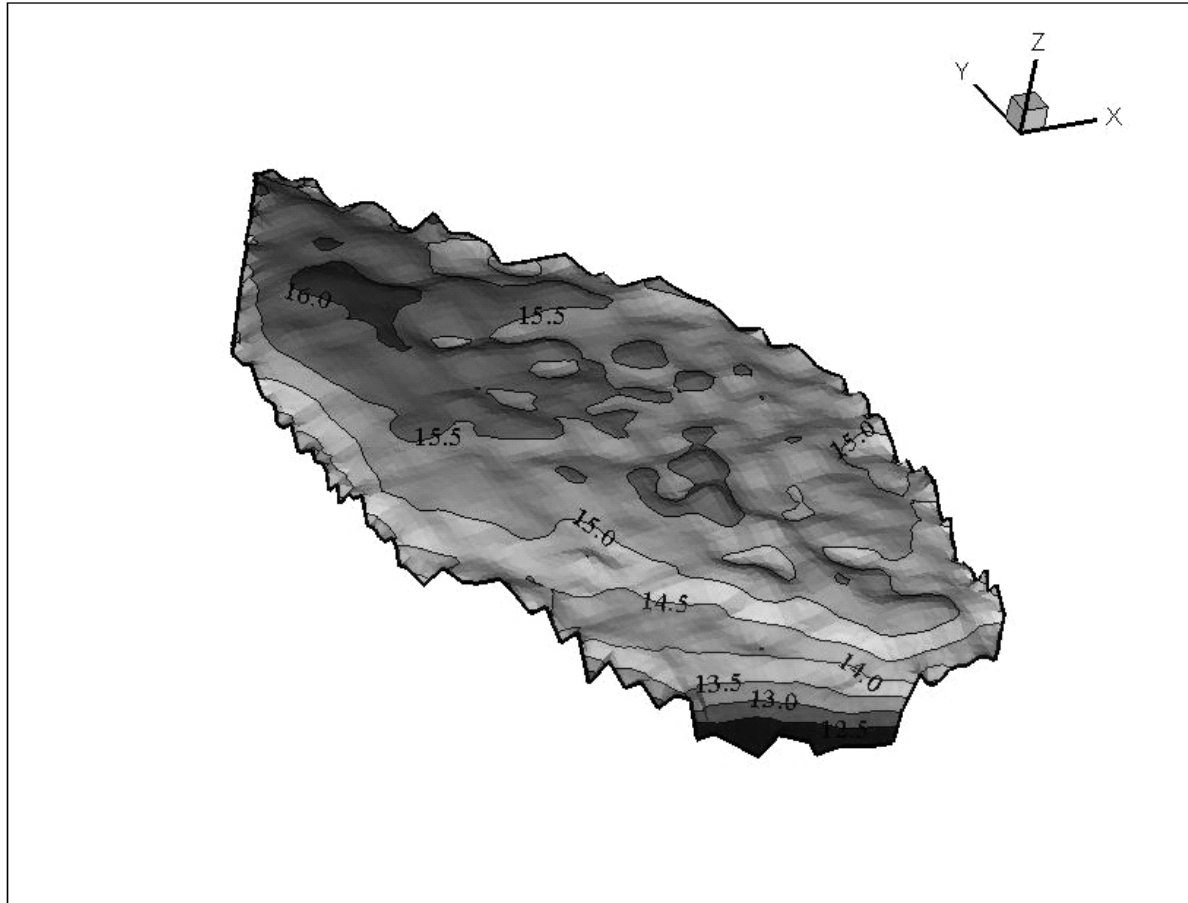


Figure 2 – Topography of the Refuge (in feet NGVD 1929) based on USGS published elevations. The site of the S-5A pump station is shown in this figure. Desmond (2003)

Perimeter canal cross-section elevation data were collected by the University of Florida's Institute of Food and Agricultural Sciences with approximate 1600 m resolution (Daroub et al., 2002) and was supplemented by measurements taken by the USFWS. The sediment surface elevation for the eastern canal (L-40) and the western canals (L-7 and L-39) vary with a mean elevation of 0.98 and 0.73 m, respectively (Meselhe et al., 2005) (Fig. 3). Water and nutrients enter and exit the Refuge through 19 hydraulic structures located around the perimeter canal. Water is pumped from inflow pump stations into the Refuge. Several

structures (S-5AS, G-301, G-300, and G-94C) are bidirectional. The largest outflow structures (S-10A, S-10C, S-10D, and S39) are located toward the southern end of the Refuge. Historical flow records for these structures are maintained by the South Florida Water Management District (SFWMD) in a publicly-available online database, DBHYDRO (http://www.sfwmd.gov/dbhydropls/sql/show_dbkey_info.main_menu).

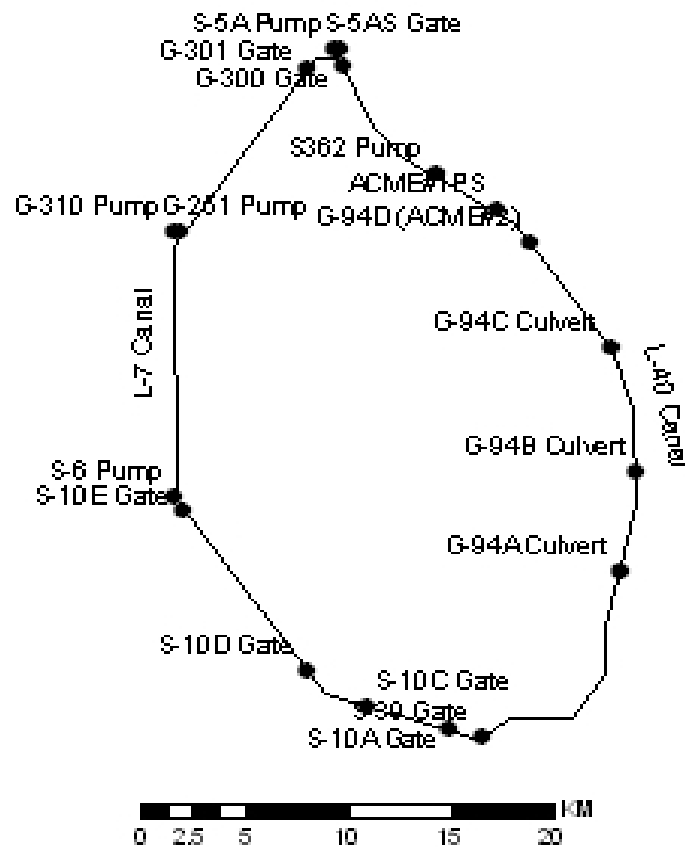


Figure 3 – Hydraulic structures in the perimeter canal of the A.R.M. Loxahatchee National Wildlife Refuge

1.3 Water Regulation Schedule

Water levels in the Refuge are managed to meet stage regulation requirements for water supply and flood protection. Regulatory releases are mandated when the Refuge stage is in a seasonally defined flood control zone defined in a Refuge Water Regulation Schedule (WRS) and is administered by the U.S. Army Corps of Engineers (USACE, 1994), Jacksonville District (Fig. 4). Regulation schedule is useful for:

- Flood Control
- Wild Life Preservation
- Water Supply
- Salt Water Intrusion

The Refuge WRS is grouped into four zones (Figure 4):

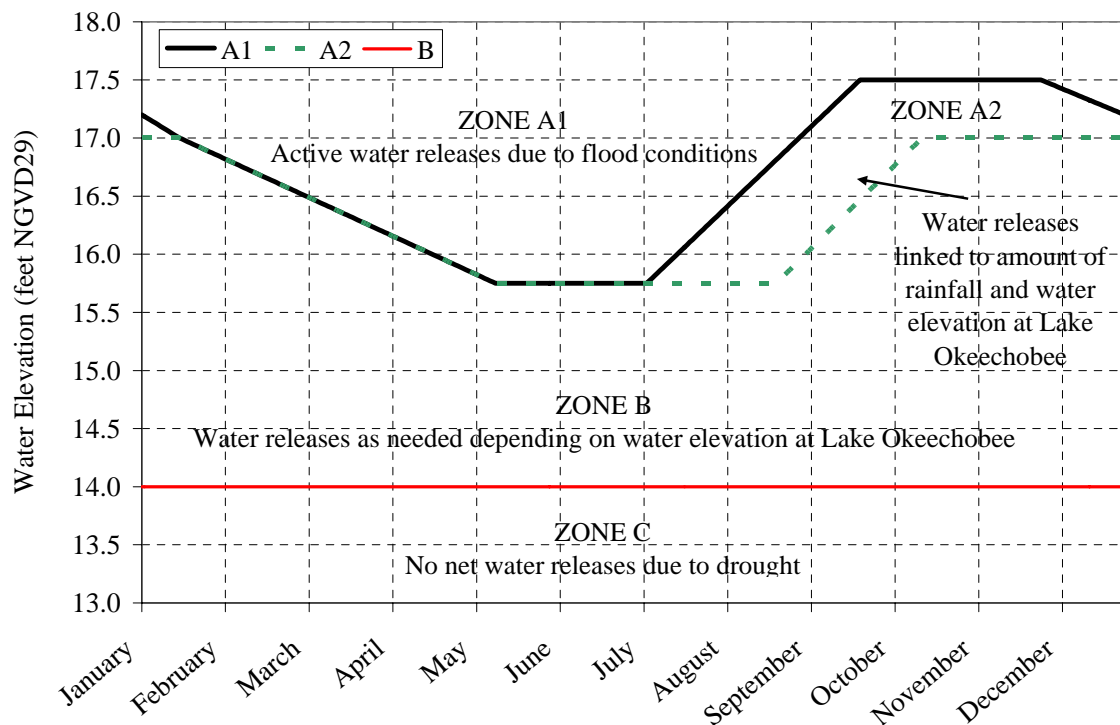


Figure 4 – Water Regulation Schedule for the Refuge. Adapted from USFWS (2000)

- Zone A1 is the flood control zone from January through June. When water levels reach this zone, active water releases will be made through the S-10 spillways (and S-39 or other structure when agreed between USACE and the SFWMD).
- Zone A2 is the flood control zone from July through December. In this zone water levels in the Refuge are permitted to reach a maximum of 5.334 m (17.5 ft) NGVD 29. Excess water is released, typically from the S-10 and S-39 spillways, based on USACE forecasts. If Lake Okeechobee's stage is above the Refuge's stage or no more than one foot below, then water supply releases from the Refuge must be preceded by an equivalent volume of inflow.
- Zone B is the water supply zone. Water levels range from a minimum of 4.267 m (14.0 ft) NGVD 29 up to a maximum of 5.334 m (17.5 ft) NGVD 29. When water levels in the Refuge are within this zone, water releases are allowed, as needed depending on the water level at Lake Okeechobee. If Lake Okeechobee's stage is above the Refuge's stage or no more than one foot below, then water supply releases from the Refuge must be preceded by an equivalent volume of inflow. This is the zone considered to be most beneficial to fish and wildlife of the Refuge (USFWS, 2000).
- Zone C is the lowest zone where water levels drop to 4.267 m (14 ft) NGVD 29 or lower. If water supply releases do occur, they must be preceded by an equivalent volume of inflow; because water levels in the Refuge interior are very low, significant attention is paid to the effects on the ecosystem when water management decisions are made in this zone.

1.4 Data Collection

The daily-averaged structural flows were obtained from DBHYDRO. Daily precipitation and evapotranspiration (ET) data from available gages were acquired from various sources (Meselhe et al., 2005). Five continuous water level stations maintained by USGS are located in the marsh, and another station (1-8C) is located in the eastern canal (L-40) (Fig. 5). All concentrations (CL, SO₄ and TP) were obtained from five data collection programs: 1) the Everglades Protection Area Project (EVPA) water quality stations; 2) enhanced water quality monitoring stations (data available after August 2004, alternatively termed LOXA or A stations); 3) SFWMD transect monitoring sites (also known as the XYZ sites); 4) water quality monitoring sites located at the structures; and 5) additional independent monitoring sites (Meselhe et al., 2005).

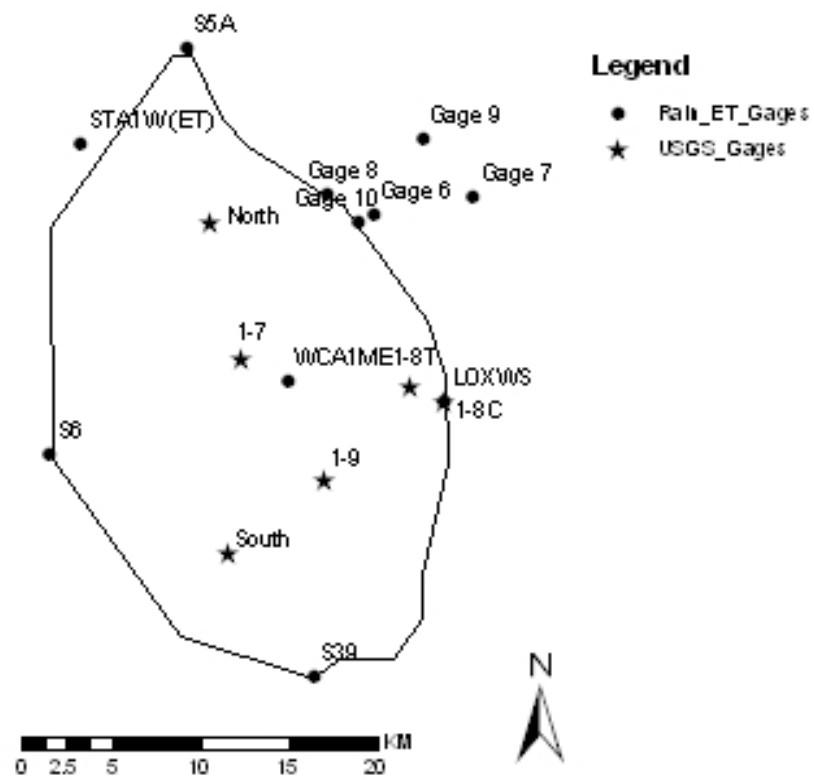


Figure 5 – Location of rain gauges, ET site and USGS water level stations in the Wildlife Refuge

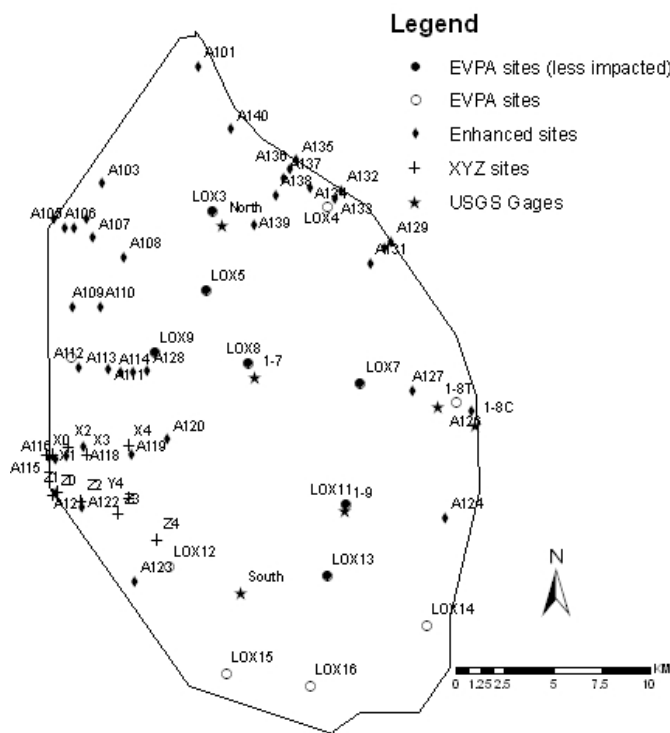


Figure 6 – Water quality monitoring stations in the Refuge

1.5 Development of the 39-Compartment Model

Water quality in the Refuge shows spatial and temporal patterns because of variations in pumped inflow and structure outflow timing, concentration, and location in the perimeter canals, as well as marsh vegetation distribution, bathymetry, rainfall, and evapotranspiration (USFWS, 2000; Arceneaux et al., 2007; USFWS, 2007a,b; Harwell et al., 2008; Surratt et al., 2008). Two alternatives for implementing large-scale wetland water-quality models involve either: (1) a spatially distributed model, or (2) spatially aggregated (lumped) model defined

by a number of compartments that are assumed to each be uniform or well-mixed (Wang et al., 2008). A water-quality model application to large geographical areas typically involves the spatial aggregation of sub-areas into compartments which are assumed within the model to be uniform (Wang et al. 2008). Alternatively, compartmental models can only detect spatial variations among compartments, and are therefore constrained by the spatial compartment boundary delineation. In general, compartments should be delineated to minimize water quality variation within each compartment, and preserve important spatial variations between compartments.

1.5.1 SRSM (Simple Refuge Stage Model)

Arceneaux (2007) implemented SRSM v1.0 4-Compartment Model (using Microsoft Excel with a daily time step. Arceneaux (2007) also implemented RWQM v1.0 (Refuge Water Quality Model) using WASP (U.S. Environmental Protection Agency's (EVPA) Water Quality Analysis Simulation Program, Version 7.1) with the same simulation periods as SRSM and driven by exchange flow from SRSM. The delineation of the 4-Compartment Model (Fig. 7) was based qualitatively on the distribution of chloride and phosphorus concentrations with distance from the canal. The first marsh compartment was within the first kilometer from the canal (0 – 1 km), the second marsh compartment was between one and four kilometers from the canal (1 – 4 km), and the third marsh compartment aggregated the remaining interior marsh area (> 4 km). The calibration period was selected as January 1, 1995, to December 31, 1999, and the validation period from January 1, 2000, to December 31, 2004.

Although SRSM can be applied to simulate a wide variety of refuge-wide scenarios (e.g. effects of effluent concentration reduction and water management alterations), it does not provide site-specific information in the results and predict North/South and West/East variations well. It also does not account for releases made for water supply or hurricane.

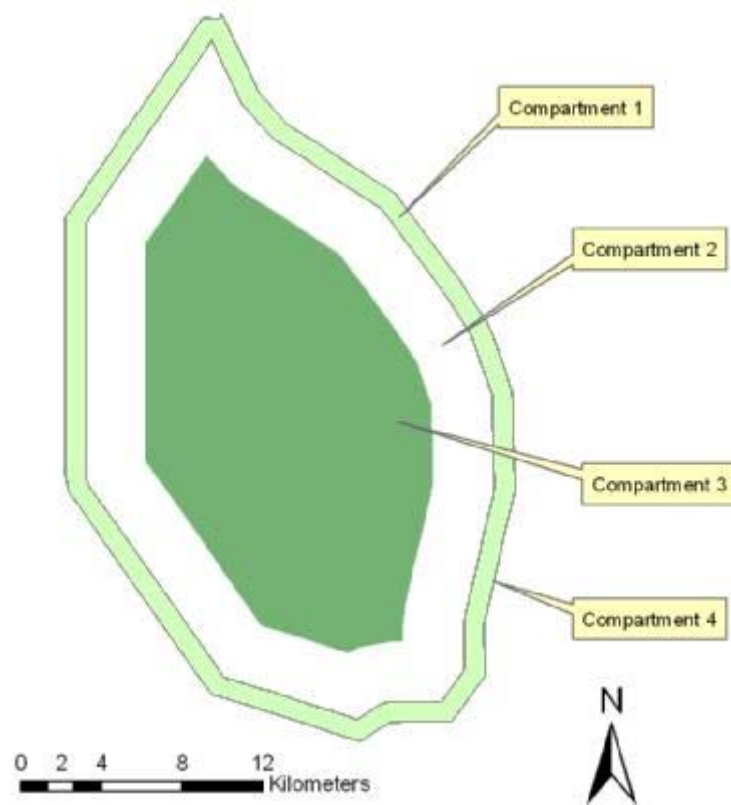


Figure 7 – Compartment delineation of the SRSM 4-Compartment Model

1.5.2 9-Compartment Model

Wang et al. (2008) applied cluster analysis (CA) to objectively determine the number of compartments and to spatially delineate compartments with similar features in the Refuge. His study was based on the analysis of concentrations of chloride, total phosphorus, sulfate,

and calcium measured at sites distributed throughout the Refuge for the period of 1995–2006. Clusters identified through CA often are highly sensitive to the variables used, and inclusion of highly correlated variables can dramatically affect cluster analysis results (e.g., Güler et al., 2002). Wang et al. (2008) used a de-correlation method (Conrads et al., 2003) for water quality parameters because Ca and SO₄ are closely related to Cl. De-correlation is accomplished by generating regression equations for Ca to Cl and SO₄ to Cl, then removing the information contained in the Cl signal from the Ca and SO₄ signals by computing the residuals (subtracting the predicted Ca and SO₄ values from actual Ca and SO₄ measurements) (Wang et al. 2008). Cluster Analysis led to the delineation of a 9-compartment model structure. The 9-Compartment Model consists of 3 canal and 6 marsh compartments. Figure 8 shows the design of the 9-Compartment Model. Even though the 9-Compartment Model represents improved spatial resolution and predictive capability for modeling the spatial variation within the refuge, it was still not adequate to analyze site specific events.

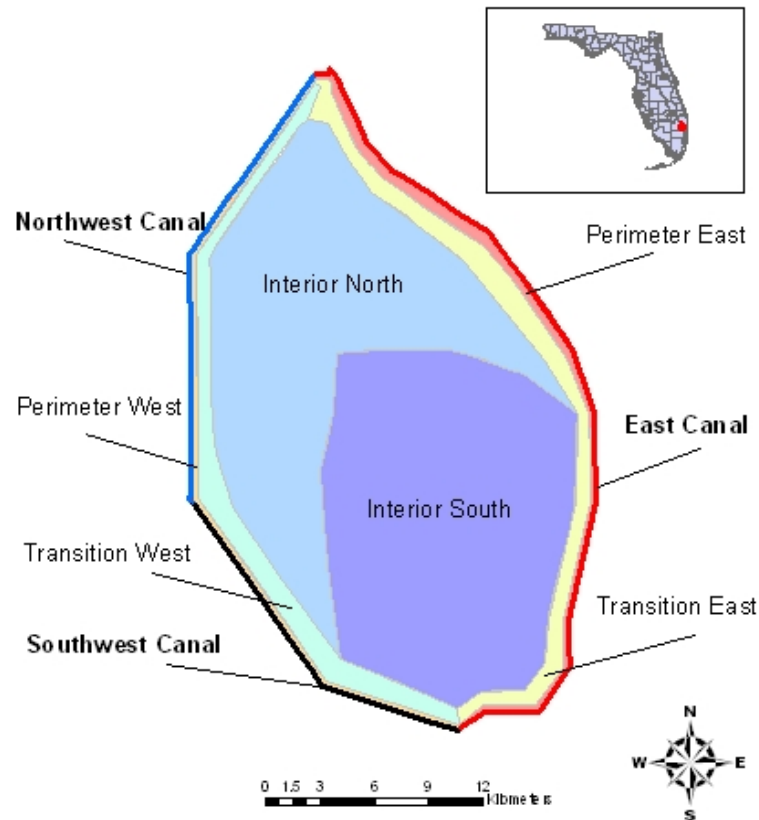


Figure 8 – Delineation of the 9-Compartment Model based on cluster analysis

1.5.3 39-Compartment Model

Spatial resolution of the 9-Compartment was not still sufficient to describe water quality gradients (North-South for canal and East-West for marsh) according to the 9-Compartment Model calibration and validation. By analyzing the water quality gradient from the calibration and validation of the 9-Compartment Model, and analyzing the vegetation/ elevation map of the Refuge, a 39-Compartment Model was built to make water exchange between compartments simple in the Berkeley Madonna model, each compartment has one connection to its neighboring N-S and W-E compartment. This delineation led to the division of the 9 compartments into 39 compartments with 11 canal and 28 marsh compartments. This

model supports investigation of the spatial details of the water and constituent movement in the Refuge. Fig. 9 shows the spread of water quality stations in the 39 compartment delineation which their observing data were applied for water quality gradient analysis.

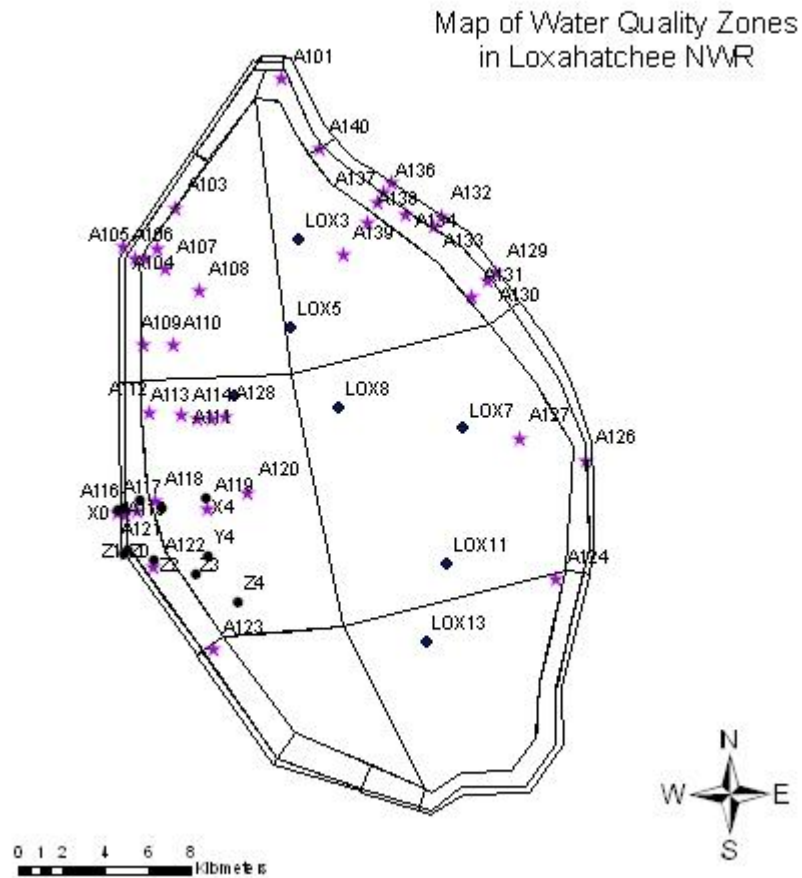


Figure 9 – Configuration of the 39-Compartment Model

Canal compartments are denoted as C, and marsh compartments are denoted as M in this document. Fig. 10 shows the location of the 39 compartments.

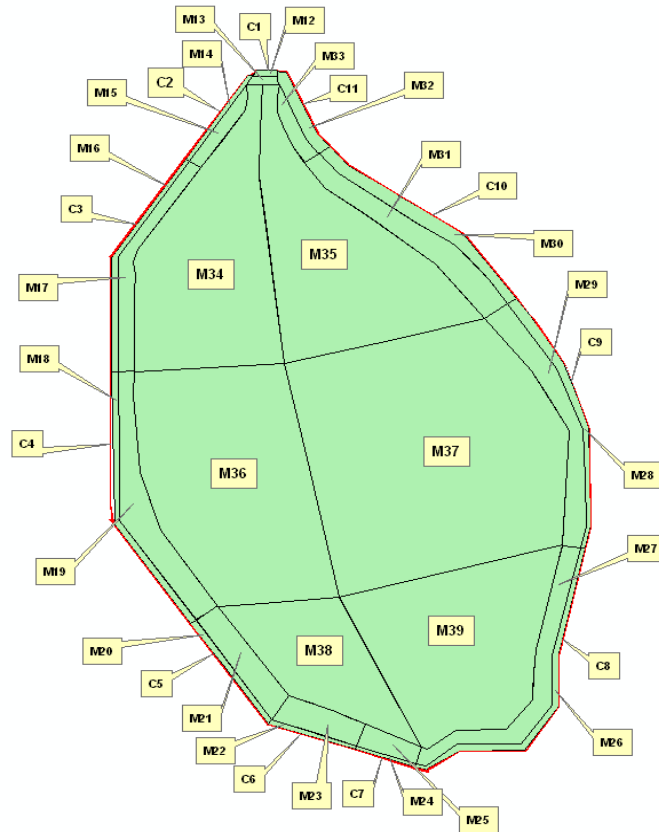


Figure 10 – The 39 compartment layout (red for canal compartments and green for marsh compartments) plotted to scale using Arc-GIS (Adapted from Shrestha, 2011)

Fig. 11 presents the link-node diagram of the 39 compartments. The figure shows the primary direction of the flow passing in/out of the neighboring compartments.

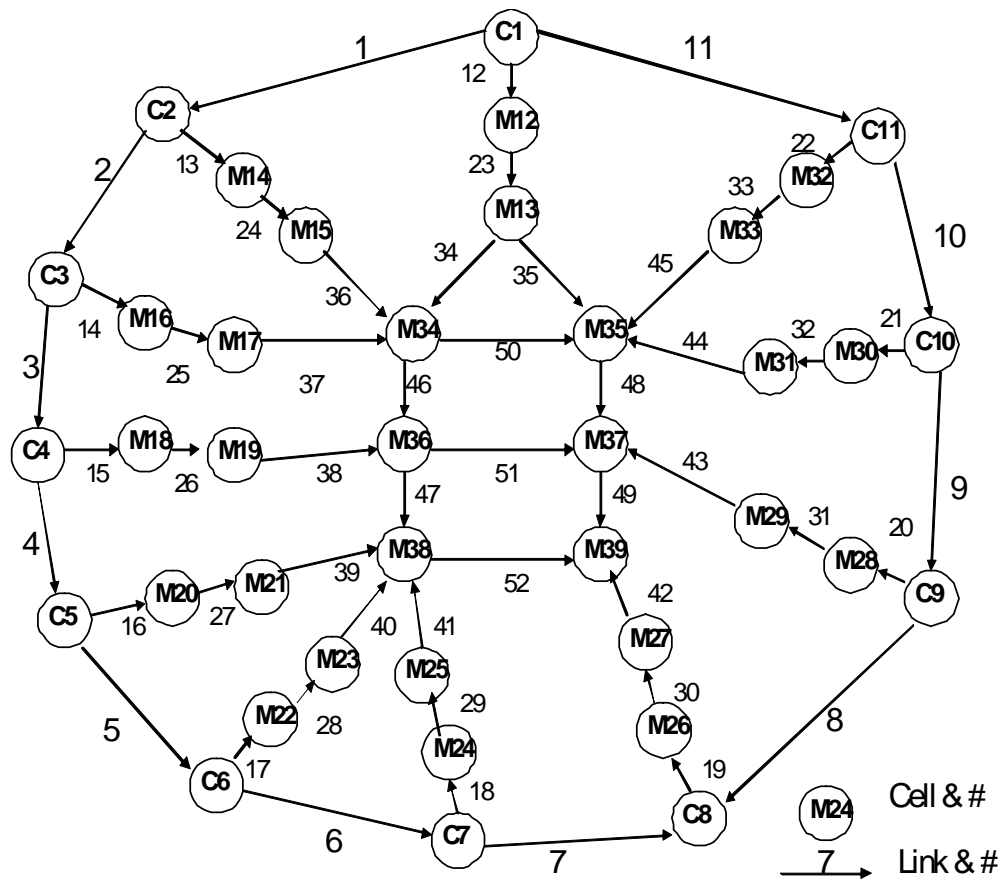


Figure 11 – Link-node diagram of the 39-Compartment Model, and the positive flow direction towards each of the two neighboring compartments. (Adapted from Wang et al. unpublished)

2 Literature Review

Regarding the 2 objectives of this thesis project, this literature review is being focused on the development of the 39-Compartment Model, along with the comparative analysis of the 39-Comapamrtmnt Model and Spatially Explicit Model.

2.1 The 39-Compartment Model

2.1.1 Compartment Modeling in Everglades

Lin (1979)

Lin (1979) adapted and modified the Receiving Water Quantity Model to model the WCAs in order to investigate the hydraulic impact of additional inflow under different pumping scenarios. Lin (1979) modeled WCAs 1, 2A, and 3A with 20 link-nodes each. The network system for WCA 1 contained 20 nodes and 57 channels. The calibration of the model was based on a comparison of predicted and observed stages at selected gages. The model was calibrated for the year 1974 and was later applied to the period 1962 to 1973. For WCA 1, modeled and observed values at gages S-6, 1-8, 1-7, and 1-9 were compared. Gages S-6 and 1-8 are located in the existing canal system, while 1-7 and 1-9 are located in the central marshland of the Refuge. For the validation period, important deviations were observed between the model results and the measurements. The deviation for interior gages was far less than that seen in the canal system. Lin (1979) recommended that the number of nodes in the network system should be increased in order to provide a better representation of the real water body. Neither groundwater nor water quality were modeled.

MacVicar et al. (1984)

MacVicar et al. (1984) presented the application of the South Florida Water Management Model (SFWMM) to two planning areas, the Lower East Coast (LEC) and the Upper East Coast (UEC). The WCA 1 was included in the LEC model that also included the other WCAs, the Everglades Agricultural Area, and some other nearby areas. A two by two mile node spacing was used to cover the 6,880 square mile area modeled. A time step of one day was used. The model was able to simulate overland, channel, and groundwater flow.

McVicar et al. (1984) indicated that simplified mathematical formulations were implemented in order to make the model computationally efficient. For example, the canal routine developed for this model was a mass balance procedure that sums all the inflows and outflows of a canal to determine the water surface position at the end of each day. The canals were defined as continuous channel reaches with flow control structures at the upstream and downstream ends. The overland flow was simplified using a diffusion flow approximation based on Manning's equation. According to MacVicar et al. (1984), the model did simulate regional flooding in undeveloped areas, and also indicated excessive groundwater drawdowns when they occurred, although it was unable to provide detailed flood routing results for single events or define detailed depression cones around municipal wells.

Kadlec and Hammer (1982) and Kadlec and Knight (1996)

Kadlec and Hammer (1982) presented a theoretical paper discussing the transport of pollutant in wetland systems. They indicated that water flow in wetlands ecosystems usually occurs in thin-sheet flows at slow rates, which are controlled by the ground slope, water depths, type of

vegetation and by the degree and type of channelization. Kadlec and Hammer (1982) indicated that removal rates in wetland systems are fast in comparison to typical biological processes, and can be represented by a first-order reaction. Kadlec and Knight (1996) also suggested nitrogen and phosphorus removal in wetland systems can be approximated by first-order models. They indicated that corrections need to be made to account for non-ideal flow, infiltration, and atmospheric inputs and outputs.

Wang and Mitsch (2000)

Wang and Mitsch (2000) used a similar model to the one presented by Mitsch and Reeder (1991) for the evaluation of phosphorus dynamics in a created riparian wetlands. The hydrology module was updated to include seepage, and bank storage in the water volume balance calculation, and periphyton community was included in the productivity model. The authors indicated that simulated TP concentrations did not follow observed data well, especially during times where there was no outflow or in low flow periods. They conjectured that it was due to the fact that the model itself is a steady-state lumped model, unable to capture influences of disturbance and random effects such as wind stirring of sediments. The lack of an atmospheric deposition term may have also introduced errors in the phosphorus budget calculations.

Raghunathan et al. (2001)

Raghunathan et al. (2001) developed the Everglades Water Quality Model (EWQM) to predict phosphorus fate and transport in the Everglades. The WCAs and the Everglades National Park (ENP) were included in the model. The output from the SFWMM was used to

transport phosphorus between model cells and canals. As in the SFWMM, the model used two-by-two mile grid-cells. A simplified relationship based on a single apparent net settling rate coefficient was used to represent the combined effect of all biogeochemical processes that control the dynamics of phosphorus in the water column. This simplified relationship indicated a net deposition of phosphorus in the sediments. An apparent net settling rate equal to 6.30 m/year was found for WCA 1 during the calibration period. The model was simulated from 1979 to 1989. Model results indicated that the interior of WCA 1 exhibits much lower concentration than the areas near the rim canal. However, the rim canal was simulated with a single water quality segment without nutrient concentration gradients (the EWQM assumed a constant canal water depth of 3 m). Model results also suggested that reduction of phosphorus concentrations leaving the EAA will result in lower concentrations entering the Everglades National Park (Raghunathan et al., 2001). It was concluded that this model proves to be a good tool for screening the effects of nutrient reduction options in the regional scenario of the EAA-WCAs-ENP system; however, it lacks the level of detail necessary to accurately model the phosphorus dynamics, and the temporal and spatial distribution of water within the Loxahatchee Refuge.

2.1.2 Previous Modeling/Studies for the Refuge

Richardson et al. (1990)

Richardson et al. (1990) studied the distribution of water over space and time and how vegetation was being structured on the Refuge by hydro-period pattern. A hydrologic model was developed to better understand the hydrologic characteristic of the Refuge. For this task, topographic data and water depths were gathered and the percent covered by each vegetation

class was recorded. A flat pool of water in the Refuge was obtained by holding water at the 17 foot level during the time that the grid survey was being conducted. Marsh soil surface elevations were determined by subtracting measured water depths at each of the grid locations from an assumed horizontal water level.

A hydrologic simulation model was constructed utilizing the Adaptive Environmental Assessment Everglades Simulation Model (AEA Everglades Model) developed by Carl Walters (Walters, 1990; Tait, 1990). Some modifications were made to the AEA Everglades model to make it applicable to the Refuge; some of these modifications included reducing the cell size, adjusting Manning's roughness coefficient, tagging cells located around the edge as canal cells, and using data from the Refuge. The stage of the rim canal was not modeled, but rather inputted as a boundary. The input and output to the canal were controlled using the historic monthly canal levels (data from SFWMD) by adjusting the water depths in canal cells.

Welter (2002)

Welter (2002) used the Regional Simulation Model (RSM) to simulate the hydrology of the Loxahatchee Refuge. The model used a grid with 16,292 triangular cells with average element size of 650 ft. Overland, canal, and groundwater flows were modeled. Welter (2002) expressed that the groundwater portion of the model was simplified as much as possible, because the overland processes seemed to be more important.

The RSM was calibrated over the period of record of 1988 to 1990, and validated for the four-year period, 1991 to 1994. The model results showed the same trends observed in the field measurements. However, some deviations were observed. Welter indicated that “the most disappointing aspect of these results is that measured data shows a larger slope in the canal’s water level than the model calculates.” He attributed this discrepancy to inaccurate cross section data which, according to Welter, overestimated depths. Welter also stated that “the limiting factor in this modeling effort is the sparse network of stage monitoring stations in the Refuge.”

Arceneaux (2007)

Arceneaux (2007) developed a water budget model for the Refuge to provide a useful tool in support of Refuge water management decisions. The water budget model was developed as a double-box model that predicts temporal variations of water level in the Refuge rim canal and marsh based on observed inflows, outflows, precipitation, and evapotranspiration and from estimated seepage rates. Chloride and phosphorus were also modeled using a 4-compartmental model coupled with the water budget model and run using the Water Quality Analysis Simulation Program (WASP 7.1). Chloride was modeled as a conservative tracer with flows determined in the Refuge water budget model. Phosphorus was modeled using the carbonaceous biological oxygen demand (CBOD) state variable to implement the k-c* model. The results for both the water budget and water quality models proved to be computationally efficient.

Wang, et al. (2008)

Wang et al. (2008) applied cluster analysis (CA) to objectively determine the number of compartments and to spatially delineate compartments with similar descriptive features for water-quality modeling. Surface-water quality data collected in the Refuge were analyzed using CA of concentrations of chloride, total phosphorus, sulfate, and calcium measured at sites distributed throughout the Refuge. Cluster analysis classified the marsh into six spatial compartments: Perimeter East; Perimeter West; Transition East; Transition West; Interior North; and Interior South. Although the perimeter canals surrounding the Refuge marsh were all connected, they clustered into three water quality compartments: Canal East; Canal Northwest; and Canal Southwest. Cluster validation criteria (pseudo F statistic and the cubic clustering criterion) indicate that there is an advantage of this new compartmental design when compared with our previous compartmentalization method that delineated boundaries using only distance from the canal to the marsh interior and professional judgment (SRSM v4). The approach provided a more technically rigorous compartmentalization for the purposes of water quality modeling. The approach supported more efficient modeling of spatial and temporal variation in water quality along the gradient from both the peripheral canal to the marsh interior, and from west to east and from north to south gradients.

Roth (2009)

Roth (2009) developed the Simple Refuge Screening Model (SRSM) version 4. SRSM was implemented using the ordinary differential equations solver Berkeley Madonna (www.berkeleymadonna.com). The compartment size and arrangement were identical to an earlier version of this model, whereas the constituent modeling approach had become more

refined. Concentrations were calculated for chloride as a conservative tracer, sulfate using a Monod relationship, and total phosphorus dynamics as described by Walker and Kadlec (2008) in the Dynamic Model for Stormwater Treatment Areas (DMSTA). Stage and constituent concentrations modeled by the SRSRM were in good agreement with the observed data for the marsh and canal areas of the Refuge. However, such a generalized scheme only allowed for average assessments of these areas as a whole. Therefore, the SRSRM had been developed as a component in a suite of models used for various applications concerned with Refuge restoration and management.

Chen et al. (2010)

Chen et al. (2010) developed and applied a spatially explicit hydrodynamic and constituent transport surface water model for the Refuge. The spatially explicit MIKE FLOOD and ECO Lab (DHI) modeling framework was used to simulate the hydrodynamics and chloride transport within the Refuge. The MIKE FLOOD model dynamically linked a one-dimensional model of the 100 km perimeter canal with a 400 m uniform grid of over 3600 two-dimensional marsh model cells, and allowed for exchange of water and constituents between the two systems. Constituent transport were driven by modeled water flows and dispersion, as constituent concentrations were transformed through reactive and settling processes which had been modeled within the ECO Lab framework. The model was calibrated for a 5-year period (2000–2004), and validated for a 2-year period (2005–2006). The graphical and statistical comparisons of stage, water depth, discharge and concentration demonstrated the applicability of the model for temporal and spatial prediction of water levels, discharge and water quality concentrations, and also demonstrate that MIKE FLOOD is a feasible alternative for modeling large wetlands that are flooded by overbank flow. The

model quantified the importance of mechanisms across the Refuge linking wetland concentration to inflow concentration and volume.

2.2 Comparative Analysis of Compartment-based Model and Spatially Explicit Model

Dai et al. (2010)

Dai et al. (2010) compared two hydrologic models with different spatial scales, MIKE SHE (spatially distributed, watershed-scale) and DRAINMOD (lumped, field-scale), in terms of performance in predicting stream flow and water table depth in a first-order forested watershed in coastal South Carolina. Model performance was evaluated using Nash-Sutcliffe Efficiency (NSE) and coefficient of determination (R^2). They found both models' performance were very good in predicting monthly and annual average water table depths and stream flow but MIKE SHE produced better results than DRAINMOD for daily hydrologic processes. The authors claimed that MIKE SHE is more robust and their predicted results are better across varying climatic conditions.

Diaz-Ramirez et al. (2010)

Diaz-Ramirez et al. (2010) compared lumped and distributed hydrologic models for the runoff simulation of a large watershed in Alabama and Mississippi. They used BASINS (Better Assessment Science Integrating point and Non-point Sources)/HSPF (Hydrological Simulation Program-FORTRAN) and WMS (Watershed Modeling System)/GSSHA (Gridded Surface Subsurface Hydrologic Analysis) to model lumped and distributed

hydrologic models. HSPF is an extensive water quality/quantity watershed model and GSSHA is a physics based multidimensional watershed model. Their main objective was to apply and test the implication of HSPF and GSSHA to estimate overland flow in the Luxapallila Creek watershed (1858 km²), situated in Alabama and Mississippi. They found that both models HSPF and GSSHA under predicted runoff during evaluated storm events. The author claimed that the GSSHA model had a better performance than HSPF runoff results when calibrated parameters were assessed in a sub-watershed outlet.

Shrestha (2011)

Shrestha (2011) focused on quantitatively comparing the 39-Compartment Model and the Spatially-Explicit Model to assess their performance. The comparison revealed varying levels of agreement among the entire 39 compartments. In general, the models were most consistent towards the northern area of the Refuge and displayed discrepancies towards the southern areas. Canal results for water stage and the constituent concentration performed well in both models. Water stage comparisons in the marsh compartments were good throughout the Refuge. However, the comparison in marsh compartments was not as favorable for the constituents. The numerical diffusion and missing topographic features were among the main contributing factors to the disagreement between the two models. His analysis showed that the two models could be used complementarily in future as they address different needs for the Refuge Management.

3 Methods

3.1 Berkeley Madonna

The 39-Compartment Model is implemented using the Berkeley Madonna (Version 8.3.9) ordinary differential equations solver, which is proprietary software developed by Robert I. Macey and George F. Oster, and can be downloaded at www.BerkeleyMadonna.com. The software has some built-in functions, components and processes, which are user-defined in the equations window. Berkeley Madonna also has integrated sensitivity, optimization, and curve-fitting features. Berkeley Madonna has 5 solutions methods available which include Euler's, Runge-Kutta2, Runge-Kutta4, Auto step size, and Rosenbrock. For the 39-Compartment Model, the Runge-Kutta4 technique was applied. Comma delimited (CSV) or tab delimited (.txt) files can be imported to Berkeley Madonna.

3.2 Water Volume and Constituents Models

To evaluate the effects of various scenarios and their impacts on the water quality within the Refuge, the 39-Compartment Model was set up to study water levels and the three constituents of chloride (Cl), total phosphorus (TP), and sulfate (SO_4). Note that TP mass is measured as phosphorus, not phosphate, and SO_4 mass is measured as sulfate, not sulfur.

Water volume change rate in canal and marsh compartments are given respectively by:

$$\frac{dV_c}{dt} = Q_{in} - Q_{out} - Q_{mc} + A_c * (P - ET_c - G_c) \quad \text{Eq.1}$$

Where: t= time (day); V_c= volume of canal compartment (m³); Q_{in}= structure inflow into refuge (m³/day); Q_{out}= structure outflow from the refuge (m³/day); Q_{mc}= water volume exchange between compartments (m³/day); A_c= canal surface area (m²); P= precipitation (m/day); ET_c= evapotranspiration from the canal compartment (m/day); G_c= groundwater seepage rate from canal compartment (m/day).

$$\frac{dV_m}{dt} = Q_{mc} + A_m * (P - ET_m - G_m) \quad \text{Eq.2}$$

Where: t = time (day); V_m = volume of marsh compartment (m³); A_m = marsh surface area (m²); ET_m = evapotranspiration from marsh compartment (m/day) and G_m = groundwater seepage rate from marsh compartment (m/day).

For exchange flow between two compartments, the compartmental model uses the Power Law relationship (Kadlec and Knight, 1996)

$$Q_{mc} = CH^3 * (E_c - E_m) \quad \text{Eq.3}$$

Where: Q_{mc}= water volume exchange between compartments (m³/day) and

$$C = \frac{B * W * 10^7}{R} \quad \text{Eq.4}$$

Where: B = transport coefficient; W= average marsh width; R= length of exchange, E_c = calculated canal stage (m) and E_m = calculated marsh stage (m)

Groundwater seepage for canal and marsh compartments is given by

$$G_i = seep_i * (E_i - E_b) \quad \text{Eq.5}$$

Where: i= marsh or canal compartment; G_i = calculated seepage rate (m/day); $seep_i$ = seepage coefficient rate (1/day) and E_b = boundary stage.

All constituents are simulated based on mass balance equation. The loading terms of the mass budget *qnet* (net mass flow in surface water (g/day)), *gload* (loss to groundwater seepage and evapotranspiration (g/day)), *sload* (net canal structure inflow-outflow loads), and *aload* (gain from wet and dry deposition(g/day)) are similar in all three constituents. However, the reactive load term *rload* (loss to storage uptake/release or reaction (g/day)) is uniquely structured for each constituent.

Chloride is modeled as a conservative constituent with zero reactive loads. Its mass is lost or gained solely through dispersion and the transport of water into or out of the system.

Therefore, the *rload* term should be ignored when chloride is considered. The amount of chloride load retained in the Refuge refers to the amount of chloride that remains in the Refuge, as well as the chloride that may have left through other means of outflow, such as groundwater seepage or transpiration (Arceneaux, 2007). As observed chloride data is taken on an irregular basis for the time of simulation, and the 39-Compartment Model uses the

constituent data value whenever there is an existing flow for the corresponding date, therefore linear interpolation was applied between missing data.

The 39-Compartment Model implements a Monod relationship to approximate SO_4 dynamics (Waldon et al., 2009). Total Phosphorus (TP) dynamics are approximated with equations adapted from those presented in the Dynamic Model for Stormwater Treatment Areas (DMSTA) developed by Walker and Kadlec (2008).

3.3 Model Setup

To simulate water stage and constituents of the Refuge in Berkeley Madonna as a mass balanced system, it is vital to study the Refuge as a closed system. Then all the volume of water flowing in the Refuge (in terms of discharge entering the Refuge in the canal, and Precipitation), and volume of water flowing out of the Refuge (in terms of discharge exiting the Refuge in the canal, evapotranspiration (ET), and ground water), and the constituents concentrations for each of these flows, are considered. Flow and concentration data are available at all inflow and bidirectional structures (Fig. 3).

3.3.1 Model Assumptions

It is assumed that each of the compartments in the 39-Compartment Model has different elevation, and flat pool for each marsh compartment. Canal surface area assumed to be constant.

3.3.2 Flow

The hydraulic structures in the canal (Fig. 3) control the flows entering/exiting the Refuge.

The records of the flow towards in or out of the Refuge are daily average value in the unit of m^3/sec . The values have to be converted to m^3/day and imported in Berkeley Madonna. There are four types of flow data used in the 39-Compartment Model. One set represents all historic inflow to the system; whereas, the rest are outflows. The three different types of outflow are: historical, water supply (S-39), and emergency hurricane release (S-10ACD). The water supply release from the S-39 structure was estimated using historical daily average supply discharge.

3.3.3 Constituents

Discrete constituents (chloride, sulfate, and TP) concentrations are recorded at the hydraulic structures in the rim canal. In the model, at each flow control structure, inflow and bidirectional, the load of each constituent is calculated when there is a flow passing at each hydraulic structure. Therefore, concentration data was interpolated linearly between each two recorded measurements at each site for chloride, sulfate, and TP before imported in the model. Grab samples are available for all three constituents (units in mg/l), whereas flow proportional composite samples are only available for TP (units in mg/l) (Roth, 2009). When available, composite values are preferred, as the sample value is assumed constant for an entire 14-day period preceding a measurement. Grab samples differ in that they occur on an irregular basis (Roth, 2009).

3.3.4 Precipitation and Evapotranspiration

Rainfall is the predominant type of precipitation in South Florida (Arceneaux, 2007). There are 9 gages used to estimate daily average precipitation for the Refuge (Fig. 5). Time series for the 39-Compartment Model represent area-averaged precipitation for each event and are constructed using the Thiessen Polygon Method, which weights the precipitation from each gage based upon its area of influence and assumes that the rainfall received at any point in the watershed is equal to that of the nearest gage (Chow et al., 1988). Thiessen Polygon Method was applied for the period of 1998–1999 and 2004–2007. For the period of 2000–2004 and 2008–2010, the daily average precipitation of the Spatially Explicit Model was used.

There is one gage used to estimate daily ET for the Refuge (Fig. 4): STA1W, formerly the ENRP area. This site directly measures ET using a lysimeter. German (2000) concludes that ET does not vary considerably across the entirety of the Everglades; therefore, it is reasonable to use a single gage reading for the Refuge. However, local effects of ET, such as vegetation type and water depth, are present across the Refuge. The potential ET was reduced in the Berkeley Madonna code when observed water depth was low using a reduction factor

of f_{ET} (Meselhe et al., 2010):

$$ET_{act} = f_{ET} * ET_{obs} \quad \text{Eq.6}$$

Where

ET_{act} = actual ET estimated from ET reduction (mm/d)

ET_{obs} = measured potential ET (mm/d)

$$f_{ET} = \max(f_{ET\min}, \min(1, \frac{H}{H_{ET}})) \quad \text{Eq.7}$$

where

$f_{ET\min}$ = minimum reduction of ET due to shallow water depth (%)

H = estimated water depth (marsh)

H_{ET} = depth above which ET is not reduced (marsh)

Table 1 shows the input files needed for the 39-Compartment Model.

Filename (alphabetical)	Summary
<i>CL.txt</i>	Chloride concentration values (mg/L)
<i>INFLOW.txt</i>	Historic inflow values (m ³ /d)
<i>OUTFLOW.txt</i>	Historic outflow values (m ³ /d)
<i>PET.txt</i>	Precipitation and Evapotranspiration (m/d)
<i>Regulation.txt</i>	Water supply release from S-39 and hurricane releases from S-10 structures (m ³ /d)
<i>SO4.txt</i>	Sulfate concentration values (mg/L)
<i>TP.txt</i>	TP concentration values (mg/L)

Table 1 – Input files for the 39-Compartment Model

4.1 Model Sensitivity

Berkeley Madonna has a feature for sensitivity test. Preliminary sensitivity tests for the 39-Compartment Model indicate that the 39-Compartment Model is sensitive to evapotranspiration (*Evap*), canal and marsh seepage coefficient (*Lseep*, and *rseep*), transport coefficient between compartments (*B* values, which represents *B1*, *B2*, and *B3* in this thesis), sulfate half saturation constant (*Khalf SO₄*), and sulfate maximum removal rate (*Kmax SO₄*), *K1* (Phosphorus maximum uptake rate), *K2* (Phosphorus recycle rate), and *K3* (Phosphorus burial rate). These parameters were then calibrated automatically (except *K1*, *K2*, and *K3*). The calibrated parameter outlined by Arceneaux et al. (2007) for the ET reduction factor (*fET_min*) was used. Table 2 shows the parameters and their values for the 39-Compartment Model. For complete list of the 39-Compartment Model and their values, one may study the 39-Compartment Manual (Meselhe et al., 2012).

Parameter	Description	Unit	Value
L seep	canal seepage constant	1/day	0.042
r seep	marsh seepage constant	1/day	0.000131527
B1	transport coefficient between canal and canal cells	1/m/day	8.7
B2	transport coefficient between canal and marsh cells	1/m/day	2.3
B3	transport coefficient between marsh and marsh cells	1/m/day	6.5
ET min	minimum ET reduction factor	-	0.2
Het	depth below which ET is reduced	m	0.25
evap	fraction of ET that is evaporation	-	0.65
kd	dispersion coefficient	m ² /day	43200
K half SO4	sulfate half saturation constant	g/m ³	1
K max SO4	sulfate maximum removal rate	g/m ² /year	14.4
K 1tp	total phosphorus maximum uptake rate	m ³ /g/year	0.1064 (EMG), 0.221 (PEW)
K 2tp	total phosphorus recycle rate	m ² /g/year	0.002 (EMG), 0.0042 (PEW)
K 3tp	total phosphorous burial rate	1/year	0.3192 (EMG), 0.6631 (PEW)
inter P	total phosphorous internal loading rate	mg/m ² /year	0
wd_cl	wet deposition, chloride	mg/L	2
dd_cl	dry deposition, chloride	mg/m ² /year	1136
wd_tp	wet deposition, total phosphorous	mg/L	0.01
dd_tp	dry deposition, total phosphorous	mg/m ² /year	40
wd_SO4	wet sulfate, sulfate	mg/L	1
dd_SO4	dry deposition, sulfate	mg/m ² /year	138.2

Table 2 – Parameter values of the 39-Compartment Model from manual calibration

4.2 Automated calibration

At the beginning of development of the Refuge compartment models, the preliminary calibration were applied by hand in a try and error basis. Then, to get the advantage of the Berekeley Madonna, features of sensitivity and automated calibration were applied for further calibration of the model parameters.

The calibrated parameters outlined by Arceneaux et al. (2007) for the SRS version 1 are: transport coefficients (**B** values), seepage rate constants (**Lseep and rseep**), and the ET reduction factor (**fET_min**). Besides, automated calibration was also applied for sulfate half saturation constant (**Khalf SO₄**), and sulfate maximum removal rate (**Kmax SO₄**).

4.2.1 Automated Calibration for Water Level or Concentration Individually

Berkeley Madonna has the automated calibration feature in which user can define the target, the range for expected calibrated value (domain), and the expected accuracy of the result. The domain here refers to a numeric interval, which the calibrated value is expected to be found based on manual calibration and professional judgment.

For automated calibration, observed data for the objective in the corresponding compartment needs to be imported in the software (for example water stage or constituent). Then, in the equation window, user needs to define the objective function for which the automated calibration is to be calculated. For the 39-Compartment Model, automated calibration is calculated based on the accumulative least absolute residual. For each observing site, the absolute residual of observed and simulated data was integrated over time using Ruge-Kutta4 time integration technique. For example, equations 8, 9, and 10 show the procedure to compute the accumulated absolute residual for sulfate in compartment 9. In specific, equation 8 calculates the absolute residual between simulated and observed value for the day for which the observed value is available for sulfate. Equation 9 differentiates the absolute residual value from equation 8 with respect to time of calibration; and equation 9 gives the initial value for the summation of the residuals.

$$\text{AbsError_9Se} = \text{ABS}(\text{Se9-Obs_9Se}) \quad \text{Eq.8}$$

$$d/dt(\text{IAE9Se}) = \text{AbsError_9Se} \quad \text{Eq.9}$$

$$\text{INIT IAE9Se} = 0 \quad \text{Eq.10}$$

After calculation of absolute residuals for each of the compartments the objective function is defined as the sum of the accumulative residuals of all associated compartments for which the observed data was imported. Equation 11, shows as example of the objective function for sulfate which includes compartments C9, M35, M37, and M38.

$$\text{SUM_IAE} = \text{IAE9se} + \text{IAE35se} + \text{IAE37se} + \text{IAE38se} \quad \text{Eq.11}$$

Seepage rate constants (*Lseep and rseep*), transport coefficients (*B* values), and *evap* (fraction of ET that is evapotranspiration) were calibrated automatically for the least residuals for water stage and chloride concentration individually. The compartments with monitored stage data available at the time of automated calibration are C9, M35, M37, and M38. Table 3 shows the hydrodynamic parameters calibrated via automated calibration for least residuals for water stage objective and their manually calibrated values.

Parameters	Description	Unit	From Manual Calibration	From Automated Calibration
L seep	canal seepage constant	1/day	0.042	0.033
r seep	Marsh seepage constant	1/day	1.31527e-4	7.555e-6
B1	Transport coef. canal and canal	1/m/day	8.73	13.31
B2	Transport coef. canal and marsh	1/m/day	2.34	4.08
B3	Transport coef. marsh and marsh	1/m/day	6.49	8.52
evap	Fraction of ET that is evaporation	unitless	0.65	0.58

Table 3 – Comparison of parameter values from manual calibration and automated calibration based on stage

As, the parameters of *Lseep*, *rseep*, *B* values, and *evap* also affect water constituent, therefore, these parameters were further calibrated automatically for chloride concentration. The compartments for which the observed data are available for the automated calibration are C3, C4, C5, C6, C7, C8, C9, C10, M17, M18, M19, M21, M23, M27, M28, M30, M31, M33, M34, M35, M36, M37, M38, and M39. Table 4 shows the parameters calibrated manually and automatically for chloride concentration and their values.

Parameters	Description	Unit	From Manual Calibration	From Automated Calibration
L seep	canal seepage constant	1/day	0.042	0.030
r seep	marsh seepage constant	1/day	1.31527e-4	3.594e-5
B1	transport coef. canal and canal	1/m/day	8.73	3.827
B2	transport coef. canal and marsh	1/m/day	2.34	1.45
B3	transport coef. marsh and marsh	1/m/day	6.49	1.83
evap	fraction of ET that is evaporation	unitless	0.65	0.52

Table 4 – Comparison of parameter values from manual calibration and automated calibration based on chloride concentration

Automated calibration was also applied for sulfate parameters *K halfSO₄* and *K MaxSO₄* with sulfate concentration as the objective. Table 5 shows the parameters *K halfSO₄* and *K MaxSO₄* calibrated automatically for sulfate concentration objective and their manual and automate calibrated values.

Parameters	Description	Unit	From Manual Calibration	From Automated Calibration
K half SO ₄	sulfate half saturation constant	g/m ³	1.00	0.699
K MaxSO ₄	maximum sulfate removal	g/m ² -day	0.039	0.075

Table 5 – Comparison of parameter values from manual calibration and automated calibration based on sulfate concentration

4.2.2 Automated Calibration for Water Level and Constituent Combined

As some of the parameters impact both water level and constituents, it is necessary to apply automated calibration based on concentration and water stage at the same time. With this regard, two applications were conducted: **a)** automated calibration for *Lseep*, *rseep*, *B* values, and *evap* for chloride and water stage simultaneously; and **b)** automated calibration for *K halfSO₄* and *K MaxSO₄* for sulfate concentration and water stage at the same time. As, explained in section 4.2.1, only 4 compartments (C9, M35, M37, and M38) had water stage observed data, therefore automated calibration for chloride/sulfate and water stage objectives combined were applied for these 4 compartments. Water stage observing sites are: 1-8C for C9, North for M35, average of 1-7, 1-8T, and 1-9 for M37, and South for M38. Constituent observing sites for sulfate and chloride are: G94B in C9, average of A138, A139, Lox3, and Lox5 for M35, average of A127, Lox6, Lox7, Lox8, and Lox11 for M37, and average of Lox12 and Lox16 for M38.

Because water level and constituent have different units, it is necessary to unify the units in the automated calibration. For this purpose, relative residual was used in which the absolute

residual was divided by the average of observations. For instance, equations 12, 13, and 14 show the equations defined for water stage for compartment 9. Among those, Eq. 12 calculates the relative residual and divide the result by the mean of observed to make it unit less; Eq. 13 defines the integration with respect to time for the accumulative residual for water stage; and Eq. 14 gives the initial value for the integration. Similarly, Equations 15, 16, and 17 show the equations defined for sulfate for compartment 9.

$$\text{relativeError_9st} = \text{ABS} (\text{E9daily}-\text{Obs_18c}) / \text{mean of observed} \quad \text{Eq.12}$$

$$d/dt (\text{IAE9st}) = \text{Abserror_9st} \quad \text{Eq.13}$$

$$\text{INIT IAE9st} = 0 \quad \text{Eq.14}$$

$$\text{relativeError_9se} = \text{Abs} (\text{se9}-\text{Obs_9se}) / \text{mean of observed} \quad \text{Eq.15}$$

$$d/dt (\text{IAE9se}) = \text{AbsError_9se} \quad \text{Eq.16}$$

$$\text{INIT IAE9se} = 0 \quad \text{Eq.17}$$

Then the overall objective function is calculated in Eq.18; given as:

$$\begin{aligned} \text{SUM_IAE} = & \text{IAE9se} + \text{IAE35se} + \text{IAE37se} + \text{IAE38se} + \\ & \text{IAE9st} + \text{IAE35st} + \text{IAE37st} + \text{IAE38st} \end{aligned} \quad \text{Eq.18}$$

Table 6 shows the parameters based on the automated calibration of water level and chloride simultaneously, and for sulfate.

Parameters	Description	Unit	From Manual Calibration	From Automated Calibration
L seep	canal seepage constant	1/day	0.042	0.048
r seep	Marsh seepage constant	1/day	1.31527e-4	8.16167e-10
B1	Transport Coef. canal and canal	1/m/day	8.73	6.97621
B2	Transport Coef. canal and marsh	1/m/day	2.34	1.13863
B3	Transport Coef. marsh and marsh	1/m/day	6.49	4.55002
evap	Fraction of ET that is evaporation	unitless	0.65	0.63
K half SO ₄	Sulfate half saturation constant	g/m ³	1.00	0.65
K MaxSO ₄	Maximum sulfate removal	g/m ² -day	0.039	0.074

Table 6 – Comparison of parameter values from manual calibration and automated calibration based on stage and chloride concentration considered simultaneously, and the same for parameters for sulfate

4.3 Simulation

The simulation period for the 39-Compartment Model is from 1/1/1995 to 12/31/2010. To let the model spin up and to eliminate the impact of the initial conditions, and at the same time considering that the validity of the observed data for the period of 1/1/1995 to 12/31/1997 was not confirmed, comparison of model results with observed data was done for the period of 1/1/1998 to 12/31/2010. Statistics tables, bar charts, and time series graphs are given in Appendix A through E. For reader's information, the 39-Compartment Model would take 25 minutes for a simulation of water stage, Cl, SO₄, and TP for 16 year (1995 to 2010).

4.3.1 Statistical Model Performance Measures

To evaluate the performance of the 39-Compartment Model, there is a necessity for statistical tools besides graphical performance/time series. For this purpose, seven statistical tools were selected to be calculated: bias, standard deviation, root mean squared error (RMSE), correlation coefficient (R), coefficient of determination (R²), variance reduction, and Nash Sutcliffe Efficiency (NSE). These statistical tools are defined as:

Bias:
$$Bias = M_{avg} - O_{avg} \quad \text{Eq.19}$$

where M_{avg} is the average simulated value and O_{avg} is the average observed value.

Standard Deviation:
$$\sigma = \sqrt{\frac{1}{N} \sum_{i=1}^N (x_i - \bar{x})^2} \quad \text{Eq.20}$$

where x represents either the observed, the simulated, or error between the observed and simulated (error=observed-simulated); \bar{x} is the mean of the simulated, the observed, or error for the entire period; and N represents the number of values.

Root Mean Square Error (RMSE):
$$RMSE = \sqrt{\frac{\sum_{i=1}^N (O_i - M_i)^2}{N}}$$
 Eq.21

where O_i represents the observed value, M_i represents the simulated value; N is the total number of values.

Variance Reduction:
$$Variance\ Reduction = 1 - \left(\frac{\sigma_E}{\sigma_O} \right)^2$$
 Eq.22

Where: σ_E is the standard deviation of the error between the simulated and observed; and σ_O is the standard deviation of the observed data.

Correlation Coefficient:
$$R = \left\{ \frac{\sum_{i=1}^N (O_i - \bar{O})(M_i - \bar{M})}{\left[\sum_{i=1}^N (O_i - \bar{O})^2 \right]^{0.5} \left[\sum_{i=1}^N (M_i - \bar{M})^2 \right]^{0.5}} \right\}$$
 Eq.23

The correlation coefficient (R) measures the linear association between the simulated and observed data. The correlation coefficient will vary from -1 to +1. -1 indicates perfect negative correlation, and +1 indicates perfect positive correlation.

Coefficient of Determination:

$$R^2 = \left\{ \frac{\sum_{i=1}^N (O_i - \bar{O})(M_i - \bar{M})}{\left[\sum_{i=1}^N (O_i - \bar{O})^2 \right]^{0.5} \left[\sum_{i=1}^N (M_i - \bar{M})^2 \right]^{0.5}} \right\}^2 \quad \text{Eq.24}$$

Nash Sutcliff Efficiency (NSE): *Nash Sutcliffe Efficiency* = $1.0 - \frac{\sum_{i=1}^N (O_i - M_i)^2}{\sum_{i=1}^N (O_i - \bar{O})^2}$ Eq.25

Note that bias, standard deviation, and root mean square error (RMSE) have units; however, correlation coefficient (R), coefficient of determination (R^2), variance reduction, and Nash Sutcliff Efficiency (NSE) are dimensionless. Each of the aforementioned measures can be used for different aspect of study. Nash Sutcliff Efficiency reflects both model bias and reduction of variance. It therefore has the value of combining these independent criteria into a single goodness-of-fit measure (Arceneaux, 2007). NSE has a maximum value of one, corresponding to a perfect fit. A value of zero indicates that the model predicts no better than simply using the average observed value. Negative NSE values are often considered to indicate that a model is not useful as a predictive tool. Nash Sutcliffe Efficiency can be problematic when applied to observations with limited variation about their mean value (Arceneaux, 2007).

5 Results

As mentioned in section 4.3, time series plots, statistics and bar charts are compiled for the model results for all compartments with available observed data. Because M21 has very few water quality observed data, statistics and time series graphs were not applied for this compartment. Due to page limitation, only selected compartments with results representing good, medium, and fair model performance are shown to demonstrate the overall model performance. All of the figures will be available in the report (Meselhe et al., 2012 (in progress)).

5.1 Water Stage Results

Statistics for water level are presented in Table 8, Appendix A. Bar charts of NSE for water stage and constituents are shown in Fig. 15, Appendix A. Selected time series graph for water stage are shown in Fig. 19 through Fig. 23 in Appendix B, for canal compartments 4, 6, 8, 9 and marsh compartment 38. Shrestha (2011) pointed out that the bathymetry in compartments 22 and 29 may not be correct and suggested for future corrections. In this study, the bathymetry of all of the marsh compartments was reevaluated, and corrections were made for those which were found to contain errors.

It is evinced that the 39-Compartment Model provides good agreement with observations. NSE varies between 0.62 and 0.86. Short canal compartment 6 on the south has a bias of -0.02m and NSE of 0.62. Longer canal compartments C4 on the west, and C8 and C9 on the east have a bias of 0.09m, 0.01m, and -0.01m and NSE of 0.69, 0.64, and 0.77 respectively.

The big interior marsh compartment 38 has a bias of 0.00m and NSE of 0.86, indicating good approximation in the compartment.

5.2 Water Quality Model Results

The statistics for the three constituents (Cl, SO₄, and TP) are presented in Tables 9, 10, and 11 in Appendix A. Bar charts for NSE, bias, standard deviation of the simulated and standard deviation of the observed for the three constituents are presented in Fig. 15 through 18 in Appendix A. Time series graphs of selected compartments for chloride, sulfate, and total phosphorus comparison are shown in Appendices C through E. It is noted that the model results are daily snap shot from the model and the observed data are daily instantaneous.

6 Discussion

By comparing the statistics of water stage and the three constituents (Cl, SO₄, and TP), (Appendix A, tables 8 through 11), it is evinced that the 39-Compartment Model predicts water stage very well. Although, the overall statistics of the constituents show a good performance of the 39-Compartment Model, water stage statistics show higher efficiency than constituents. Overall the model performance for canal compartments for water stage is good. By comparing canal compartments on the west and the east side of the Refuge, it is concluded that canal compartments of 8, 9, and 11 on the east side (bias 0.01m, -0.01m, and 0.06m), have overall less bias than the canal compartments of 2, 3, 4, 5, 6, and 7 on the west side (bias of 0.04m, 0.05m, 0.09m, 0.02m, -0.02m, and 0.05m). The standard deviations of the simulated values are closer to the standard deviations of the observed on the east side. For NSE, east and west sides have roughly equal performance. Compared to the water stage data available to the canal compartments, the monitoring stations in the marsh is scarce (9 out of 11 canal compartments have observed data, while only 3 out of 28 marsh compartments have observed data).

For constituents, the overall model performance is good. The NSE for all constituents for canal compartments is positive except for canal compartment C9 with NSE of -0.01. Canal compartments 3, 6, and 9 can be considered as representative of good, medium, and fair performance for chloride. Large bias of C3 is -10.20 mg/l, with NSE of 0.50, medium bias of C9 is 6.08 mg/l with NSE of 0.29, and small bias of C6 is -3.15 mg/l with NSE of 0.47 (Appendix C, Figures 24, 25, and 26). For sulfate, C3 has a small bias of -1.00 mg/l and NSE of 0.70; while C8 has larger bias of -7.84 mg/l and NSE of 0.33 (Appendix D, Fig. 32 and

Fig. 33). For TP, C4 and C9 are selected as good and fair simulated compartments. (Appendix E, Fig. 36 and Fig. 37).

For the marsh, by studying the bar charts for NSE, bias and standard deviation for the three constituents (Appendix A, Fig. 15 through Fig. 18), it is seen that the overall model performance is good. But the three constituents perform differently. For chloride, M30 and M38 have high (0.42) and low (-1.56) NSE, and similarly for bias (-8.36 mg/l and 20.40 mg/l) (See Appendix C, Fig. 29 and Fig. 31 for time series of M30 and M38). For sulfate M18 with NSE of -0.49 and bias of -19.98 mg/l, and M30 with NSE of 0.68 and bias of 0.06 mg/l represent fair and well predicted compartments (See Appendix D, Fig. 34 and Fig. 35 for time series). For TP, M28 with NSE of -3.92 and bias of 0.092 $\mu\text{g/l}$, and M31 with NSE of 0.26 and bias of -1.268 $\mu\text{g/l}$ represent well and fair predicted compartments (See Appendix E, Fig. 38 and Fig. 39 for time series).

In specific, for chloride in M28, time series (Appendix C, Fig. 28) evinces that the model follows the observation of site Lox 6 but deviates from the site of A126. For the negative NSE for three constituents in M28, it is noted that this compartment is located at peripheral marsh where strong hydrodynamic gradient exists due to the dramatic change in bathymetry and vegetation in this compartment which makes it challenge for the 39-Compartment Model to capture the exchange of flow between canal compartment 10, marsh compartment 28 and transitional marsh compartment 29. There are discrepancies in M37 and M38 (See Appendix C, Fig. 30 for chloride time series graphs for marsh 37 and Fig. 31 for chloride time series graphs for marsh 38). The observed data in these two compartments have slight difference in

magnitude. This is because the interior marsh compartments have much larger area, and the few observing sites can not fully represent the changes of topography, hydrodynamic, and water quality characteristics within these compartments.

By studying the statistics for chloride, sulfate, and TP (Appendix A, Tables 9, 10, and 11), it is noted that the model provides better approximation in the north than in the south in general. This can be attributed that the inflow structures are all located in the north Refuge, and these structures directly impact the water and constituent movement in the northern canal and the exchange with the northern marsh area. While moving towards the south, the flow conditions become complicated as the inflows, outflows and exchanges act together.

7 Conclusions

Generally, compartment-based models are more computationally efficient, easier to use and faster to run compared to spatially explicit models. This is confirmed by the 39-Compartment Model developed in this thesis. As an example, for a 10 year simulation run it would take roughly 15 minutes for the 39-Compartment Model and 15 hours for the Spatially Explicit Model (Mike Flood) to accomplish.

The 39-Comartment Model predicts water stage very well for canal and marsh. The model also predicts the concentration of three constituents (Cl, SO₄, and TP) reasonably well, but with less accuracy compared to water stage. It is evinced that in the Refuge, the inflow structures in the north have strong impact to the flows in the canal and the northern marsh. Therefore, the model prediction in the north is overall more accurate than in the south.

The dramatic variation in the observed data for the marsh compartments of M28, M37, and M39 indicates that the design for these compartments can be improved. It is seen that the model simulations for these compartments followed the patterns of some of the observing sites. Consequently, we could say the model has the capability to predict well the water quality constituents. As these compartments contain dramatic variation in local characteristics, further compartment disaggregation based on the analysis of topography, vegetation, and special features would be expected to improve model prediction. For the peripheral marsh compartment M28, a strong hydrodynamic gradient exists due to the dramatic change in bathymetry and vegetation within the compartment.

As TP concentration is relatively low in comparison to chloride and sulfate concentration (max average of observed is 68 $\mu\text{g/l}$ in C10), by a relatively big change of observed data from the mean of observed, the denominator in NSE formula (Eq. 25) will have large deviations, and this causes NSE gets lower values, despite of having relatively a very low bias (like in M28 with the most negative NSE -3.92, but at the same time with minimum bias to be 0.092 $\mu\text{g/l}$); therefore NSE is not a practical statistical measure for evaluating TP simulation. By studying bias, standard deviation of model results, and standard deviation of observed data for TP, it is concluded that although the 39-Compartment Model predicted observed data amazingly well with small bias, standard deviations of model results have noticeable deviation from the standard deviations of the observed. This suggests that the 39-Compartment Model may have difficulty in modeling of TP.

Automated calibration of the seepage coefficients for the marsh and the canal (***rseep*** and ***Lseep***) revealed that the seepage loss in canals for the 39-Compartment Model is larger than that for the 9-Compartment Model. Although, the transport coefficients (***B*** values) were expected to have larger impact on water stage than water quality, automated calibration showed that water stage is less sensitive to the ***B*** values. However, chloride concentration is more sensitive to the ***B*** values. Because by moving the water from a compartment to another (***B*** values) with different type (canal to marsh and vice versa), part of chloride concentration is lost to seepage. As, canal and marsh have different seepage constants and the rate of absorption are different in them, the chloride concentration is sensitive to ***B*** values.

The change of stage with respect to volume for the canal compartments in the SRSM is based on a rectangular cross section assumption. Such assumption prevents the catch of low water stages. The 39-Compartment Model employed a more realistic stage-volume relationship, which is derived from the canal geometry, for the canal compartments, thus improved the water stage prediction in the case of low values.

Table 7 shows the SRSM water stage statistics for Jan 1st 1995 to Dec 31st 2004 for both the canal and the marsh compartments (Adapted from Arceneaux, 2007). Comparing it with the 39-Compartment Model (Appendix A, Table 8), it is seen that the 39-Compartment Model has the same magnitude of bias for 6 out of 12 compartments; but the 39-Compartment Model has better NSE in canals and marshes. Overall, the 39-Compartment Model performs better than SRSM for water level.

Statistical Parameter	Canal Statistics	Marsh Statistics
Bias (m NGVD 29)	0.00	-0.02
RMSE (m NGVD 29)	0.15	0.08
Standard Deviation of Observed (m NGVD 29)	0.25	0.15
Standard Deviation of Modeled (m NGVD 29)	0.23	0.17
Standard Deviation of Error (m NGVD 29)	0.15	0.08
Variance Reduction	66.9 %	73.3 %
R (Correlation Coefficient)	0.823	0.895
R ² Value	0.678	0.800
Nash Sutcliffe Efficiency	0.669	0.713

Table 7 – Marsh and canal water stage statistics for SRSM (Adapted from Arceneaux, 2007)

For SRSM, it was concluded that the marsh performed slightly better than the canal for water stage (Arceneaux, 2007). For the 39-Compartment Model, it is evinced that the model has equal performance for the canal and the marsh.

As the 39-Compartment Model represent the Refuge in higher spatial resolution than SRSM, especially along the transitional zone of the marsh, it can be used to better detect water quality variations along the western and eastern gradients. Due to the spatially-aggregated compartment design of the model, it should not be used to analyze site specific events.

The 39-Compartment Model still contains sources of uncertainties in bathymetry, inflows, rainfall, ET, and inflow concentrations. Additionally, low frequency of monitoring data, and the spatial resolution pose limitations to this model from exploring site specific events.

Some suggested future areas of investigation include:

- The discrepancies in the simulated results vs. observed data for constituents in transitional marsh compartment M19, peripheral marsh compartment M28, interior marsh compartments of M37 and M39 indicate that further compartment division may be applied for these compartments.
- Considering the substantial variation in elevation, vegetation, and soil properties in the marsh near the canal, additional surveyed information regarding these concerns would be beneficial for future modeling study.
- Also it would be helpful for future modeling study if more frequent water quality data sampling would be achieved.
- Additional constituents like carbon and total nitrogen can be added to the model to better analysis of the Refuge.

9.1 Introduction

Hydrodynamic and water quality models provide the predictive tools needed for management and scientific support. A calibrated hydrodynamic and water quality model provides managers and planners with information on movement of water, and the fate and transport of constituents (Kadlec and Hammer, 1988; Tsanis et al., 1998; Koskiaho, 2003). Models create the basis for answering questions regarding the hydrologic, hydrodynamic, and water quality conditions occurring under present conditions and management rules, and models project how these processes would be altered by alternative structural changes and management scenarios. The SRSM, the 39-Compartment Model, and the Spatially Explicit model have been calibrated and validated against measured data (Meselhe et al., 2010; Roth et al., 2009; Meselhe et al., 2011 (in press); Chen et al., 2010), and some of them have been applied to assess management scenarios (Roth et al., 2009; Chen et al., 2010). They can provide information about the response of the Refuge to hydrological and meteorological boundary conditions enforced. They also prove to have the capability of projecting the response of the Refuge to external management alterations through imposed changes in boundary flows and concentrations. Even though each model has been calibrated and validated extensively, the comparison of model performance between the compartmental model and the spatially explicit model with observed data is a topic of interest. As a continuation of Shrestha's work (2011), this topic is more fully examined and documented in this chapter. The primary objective of this effort is to compare the 39-Compartment Model and the Spatially Explicit Model for predicting water level and chloride in the Refuge. With this regard, these two

models are compared with observed data, and their performances are quantitatively evaluated. Such comparison would be useful for future modeling efforts as to how different models can be utilized complementarily (Shrestha, 2011).

The 39-Compartment Model was developed using the commercial numerical differential equation solver package of Berkeley-Madonna for predicting water level and three constituents (Chloride, Sulfate, and Total Phosphorus). The spatially explicit model was built based on the MIKE FLOOD and ECO Lab modeling framework (DHI) to simulate hydrodynamics and transport of the three constituents (Chen et al., 2010). MIKE FLOOD is a physically-based, distributed hydrological and constituent transport model. It dynamically integrates a two-dimensional grid (MIKE 21) and a one-dimensional channel flow simulation tool (MIKE 11) through user defined links (DHI, 2008) at the interface.

The model comparison study conducted by Shrestha (2011) compared the simulation results of the two models. It is recognized here that to assess the performance of these two models, it is also necessary to compare the model results with observed data. This provides a direct evaluation of the performance of each individual model (Shrestha, 2011). In this effort, the comparison of model results with observations were quantified using the statistical measures described in section 4.3.1 for chloride concentration.

9.2 Comparison Methodology

In performing model comparison, three approaches were utilized. These approaches are here termed the Aggregated Site Comparison (ASC), the Individual Site Comparison (ISC), and the Mesh Average Comparison (MAC). To examine the models' capability to capture the gradient of chloride variation towards the interior from the canal, two transects were chosen, one on the east and the other on the west side of the Refuge. Each transect starts from a canal compartment, going through a peripheral marsh compartment, a transitional marsh compartment towards an interior marsh compartment (Fig. 12). Such design was to provide information on the performance of the two models on each side, and help to better understand the canal water movement and intrusion. Another reason for choosing these two transects is that there are relatively abundant observing sites within these two transects, which provide sufficient data to facilitate the evaluation of model performances. Specifically, there are three stations in each canal compartment; and three to sixteen for the marsh compartments.

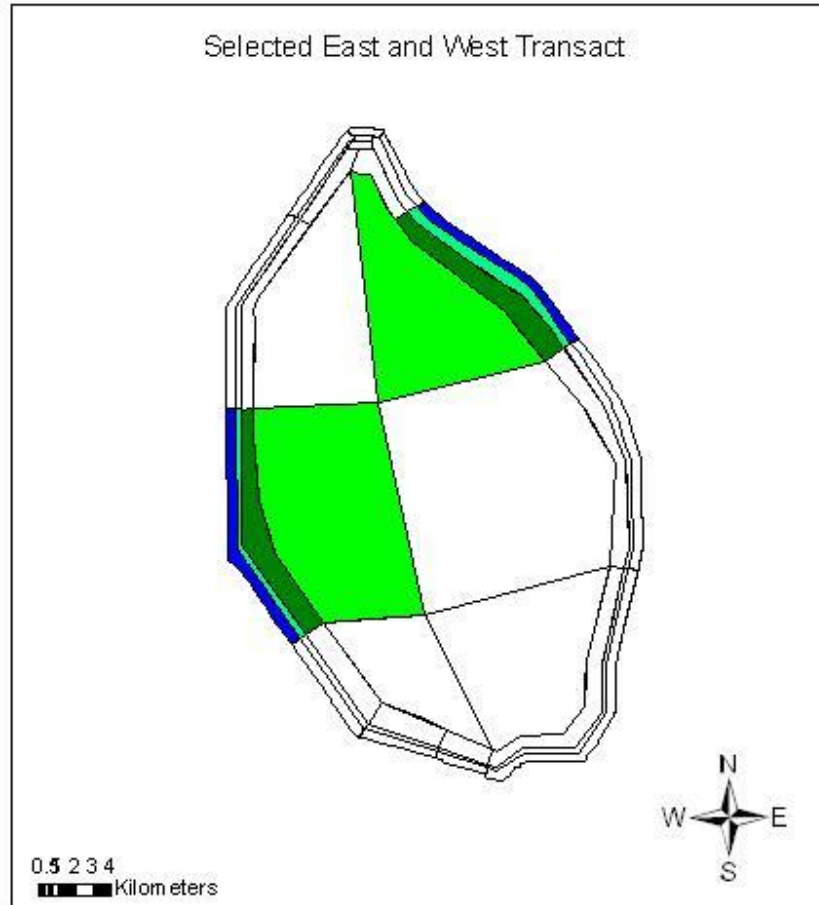


Figure 12 – Selected east and west transacts for model comparison

9.2.1 Aggregated Site Comparison (ASC)

In this approach, all the observed data of the monitoring sites that fall within one compartment were compared to the simulated value of that compartment of the 39-Compartment Model for the corresponding date. For the Spatially Explicit Model, simulated values of each individual site were compared with the observed data for the corresponding site and date.

9.2.2 Individual Site Comparison (ISC)

In this approach, the observed data from each site was compared to the simulated value of the 39-Compartment Model for the corresponding date; and with the simulated grid value of the Mike Flood model for the corresponding date.

9.2.3 Mesh Average Comparison (MAC)

In this approach, all the observed data from the sites which fall into one compartment were compared to the average of the simulated grid values of the Mike Flood model, which falls into that compartment for the corresponding date. This methodology uses an average of grid cells which is conceptually comparable to the compartment model.

9.3 Results

The statistics of bias, Root Mean Square Error (RMSE), Variance Reduction, Correlation Coefficient (R), Coefficient of Determination (R^2), and Nash-Sutcliffe Efficiency (NSE) for each compartment along the transacts were calculated for the three approaches described above. The results are given in Appendix F, tables 12 through 19. It is noted that the unit for concentration is mg/l.

9.4 Discussion

Comparison between compartments is challenging due to a number of factors including inequality in the number of observing sites in each compartment, inequality between the number of observed data for two compartments, the location of the site in the compartment and how well that site could be representative of that compartment, inequality between compartment areas, vegetation map, soil type, etc. It is also notable that this comparison is between instantaneous data (observed) with daily snap shot (simulated), and hence observed data may have a phase shift in time for some factors. Inspecting the overall compartment comparisons revealed that in some of the compartments, both models could predict observed data reasonably well (for example, C4 in table 1, M19 in table 3, C10 in Table 5, M30 in table 6, and M31 in table 7 of Appendix F). In some compartments both of the models, shows good prediction (for example, M18 in Table 2, M36 in table 4, and M37 in Table 8 of Appendix F).

It is recognized that comparison of statistics for constituents between each two sites/compartments based solely on Nash Sutcliff Efficiency may not be suitable; because according to the Nash Sutcliff Efficiency formula (Eq. 23), for sites/compartments with low observed averages, by a relatively big change of observed data from the mean of observed, the denominator in NSE formula (Eq. 25) will have large deviations, and this causes NSE to get lower values, despite of having relatively a very low bias. For values with relatively higher observed averages, the deviations of observed from the mean will have less impact on the denominator in NSE; therefore, NSE cannot be the only practical statistical measure for evaluating constituents simulation.

9.4.1 Aggregated Site Comparison (ASC)

By studying the statistics of the two canal compartments of C4 and C10, it is seen that the Spatially Explicit Model has less bias (3.09 to -5.13 in C4, and -3.83 to -11.17 in C10), and higher NSE (0.73 to 0.66 in C4, and 0.31 to 0.28 in C10) than the 39-Compartment Model. But the 39-Compartment Model has less standard deviation (37.22 to 42.19 in C4, and 26.93 to 37.56 in C10). Consequently, in the ASC method, the Spatially Explicit Model performs better for canal.

The two peripheral marsh compartments of M18 and M30 on the west and east of the Refuge perform differently. For cell 18, the Spatially Explicit Model has less bias (12.76 to -32.62) and higher NSE (0.60 to -0.18) than the 39-Compartment Model; but the 39-Compartment Model has less standard deviation (28.79 to 40.31). On the east side, the 39-Compartment Model has better performance with less bias (-8.36 to -15.11) and standard deviation (19.97 to 27.04), and higher NSE (0.42 to 0.33) than the Spatially Explicit Model. Therefore, for the west side, the Spatially Explicit Model has better performance; while on the east side, the 39-Compartment Model predicts chloride concentration better.

In transitional marsh cells of M19 and M31, the 39-Compartment Model performs significantly better for both compartments for almost all the statistics. Bias are 4.44 to -8.57 for M19, and -5.05 to -10.18 for M31. Standard deviations are 29.04 to 41.53 for M19, and 18.03 to 24.66 for M31. For NSE, on the west side, the 39-Compartment Model performs better (0.53 to 0.29), and on the east side the Spatially Explicit Model performs better (0.24

to 0.19). Therefore, the 39-Compartment Model performs better for ASC in transitional marshes.

For the interior marsh compartments of M36 and M35, the statistics are similar for the two models. Bias are -0.75 to 2.23 for M36, with the Spatially Explicit Model performs better, and -4.82 to -5.17 for M35 where the 39-Compartment Model has less error. In case of standard deviation, the 39-Compartment Model has less value with 19.17 to 20.51 for M36, and -4.82 to -5.17 for M35. For NSE, the Spatially Explicit Model performs slightly better, with values of -0.57 to -0.48 for M36, and -0.38 to 0.10 for M35. Overall, the Spatially Explicit Model has better performance for the ASC method in the interior marsh compartments.

9.4.2 Individual Site Comparison (ISC)

Because the number of observing sites are different in majority of canal and marsh compartments, and also the total number of observing data for their calculated statistics are different, for this method, the overall comparison of the sites is being discussed and the actual simulated values are not presented here (See Appendix F, table 1 through 8, for the statistics of the two transacts).

By comparing the statistics using this approach, one can recognize that for both canal compartments C4 and C10, the Spatially Explicit Model performs better in terms of bias, and NSE; but the 39-Compartment Model has lower standard deviation of simulated.

For the two peripheral marsh compartments of M18 and M30, similar to those obtained from the Aggregated Site Comparison method; the two eastern and western compartments perform differently. On the east side for M18, the 39-Compartment Model has less standard deviation; while the Spatially Explicit Model performance is much better for bias and NSE. On the west side for M30, the 39-Compartment Model performance is much better. In comparison of these two compartments, it is of interest that the average of observed of M18 is higher than that of M30. This difference will make comparison between NSE less reliable (See section 8.5 for the discussion for comparison NSE between 2 data with different average of observed.)

In transitional marsh of M19 and M31, the 39-Compartment Model has less bias and standard deviation. The NSE for the two models differs from east to west. For M19 on the west side, the 39-Compartment Model has completely better performance. On the east side, the results vary. Overall, the 39-Compartment Model performs better.

By studying the statistics of the interior marsh compartments of M36 and M35, it is concluded that for M36 on the west, the 39-Compartment Model has better performance for bias and NSE, but the Spatially Explicit Model has less standard deviation. For M35, the 39-Compartment Model has less bias, and the Spatially Explicit Model has less standard deviation. Both of the models have comparable performance for NSE. The Spatially Explicit Model has less standard deviation on both of the compartments, which confirms this model is predicting better for big interior marsh compartments.

9.4.3 Mesh Average Comparison (MAC)

In both the canal compartments of C4 and C10, MAC has the least bias than ASC for the Spatially Explicit Model and for the 39-Compartment Model (2.44 to 3.09 and -5.13 for C4, and -3.29 to -3.83 and -11.17 for C10, respectively). Comparing MAC with ASC for the two models indicates that ASC for the 39-Compartment Model has the least standard deviation (37.29 to 41.95 and 42.19 for C4, and 26.93 to 36.71 and 37.56 for C10) than MAC and ASC for the Spatially Explicit Model respectively. For NSE, MAC has the highest value (0.75 to 0.73 and 0.66 for C4, and 0.33 to 0.31 and 0.28 for C10) than the ASC method for the Spatially Explicit Model and the 39-Compartment Model, respectively.

In the peripheral marsh compartment of M18, this method performs much better than ASC for both the 39-Compartment Model and the Spatially Explicit Model. Comparing bias, MAC has the least value (7.93 to 12.76 and -32.62) than ASC for the Spatially Explicit Model and the 39-Compartment Model respectively in M18. For the other peripheral marsh compartment of M30, likewise, MAC has the least value of bias (0.97 to -8.36 and -15.11) than ASC for the 39-Compartment and the Spatially Explicit Model. Comparing the standard deviation, ASC for the 39-Compartment Model has the least value for both peripheral marshes (28.79 to 40.31 and 40.74 in M18, and 19.97 to 27.04 and 32.17 in M30) than ASC for the Spatially Explicit Model and MAC. In NSE comparison, the results differ from west to east. On the west side in M18, MAC has the highest value with 0.69 to 0.60 and -0.18, than ASC for the spatially Explicit Model and the 39-Compartment Model. On the east side of the Refuge, ASC for the 39-Compartment Model has the highest NSE with 0.42 to 0.33 and 0.28 than ASC for the Spatially Explicit Model and MAC.

In the transitional marsh of compartment M19, ASC for the 39-Compartment Model has the least bias (-4.44 to 8.57 and -8.75) than ASC for the Spatially Explicit Model and MAC sequentially; and again for M31, ASC for the 39-Compartment Model has the least error (-5.05 to -9.63 and -10.18) than MAC and ASC for the Spatially Explicit Model. In comparison of standard deviation in transitional marshes, ASC for the 39-Compartment Model has the least simulated value (29.04 to 29.66 and 41.53 in M19, and 18.03 to 22.35 and 24.66 in M31) than MAC and ASC for the Spatially Explicit Model. For NSE comparison, on the west side in compartment M19, ASC for the 39-Compartment and MAC have the same value of 0.53 comparing to 0.29 for ASC for the Spatially Explicit Model. On the east side in marsh compartment M31, MAC has the highest NSE (0.25 to 0.24 and 0.19) than ASC for the Spatially Explicit Model and the 39-Compartment Model respectively.

In the interior marsh compartment of M36, ASC for the Spatially Explicit Model has the least error (-0.75 to 2.23 and -6.59) than ASC for the 39-Compartment Model and MAC. In the interior marsh compartment of M35, ASC for the 39-Compartment Model, has the least bias (-4.82 to -5.06 and -5.17) than MAC and ASC for Spatially Explicit Model. Comparing the standard deviations for the interior marsh compartments, MAC has the least standard deviation (12.95 to 19.17 and 20.51 in M36) than ASC for the 39-Compartment Model and the Spatially Explicit Model. For the interior marsh compartment of M35, ASC for the 39-Compartment Model has the least standard deviation (11.29 to 11.78 and 15.83) than MAC and ASC for the Spatially Explicit Model. Comparing NSE in interior marsh compartments, MAC has the highest NSE value (-0.19 to -0.48 and -0.57) than ASC for the Spatially Explicit Model and the 39-Compartment Model in M36. In M35, ASC for the spatially

Explicit Model has the highest NSE (0.10 to -0.21 and -0.38) than MAC and ASC for the 39-Compartment Model.

9.4.4 Overall Comparison Methods

By studying the statistical results for the three methods, it is of concern to choose which model has a statistically better performance in each of the type compartments (canal and marsh). In canal compartments, MAC for the Spatially Explicit Model produces the best statistics. In peripheral marshes also, MAC for the Spatially Explicit Model has the best performance. Therefore, Mike Flood has a better performance for canal and peripheral marsh compartments. In transitional marshes, ASC for the 39-Compartment Model showed better statistics. Consequently, the 39-Compartment Model predicts better for transitional marshes. For the interior marsh compartments, on the west side MAC for the Spatially Explicit Model, and on the east side ASC for the Spatially Explicit Model have shown better statistics. Hence, for the interior marsh compartments, the Spatially Explicit Model predicts better.

To evaluate the overall performance of the Spatially Explicit Model, the 3-point moving averages were calculated for average and standard deviation of the observed and the simulated on both transects, and plotted with respect to the distance from the canals (figure 10 and 11). By studying the plotted graph, it is concluded that the Spatially Explicit Model provides good approximation to the observed data.

Shrestha (2011) found that good result agreements were seen in the canal compartments of C1, C2, C3, C4, C5, C9, C10 and C11, and the marsh compartments of M16, M17, M18,

M21, M33 and M34 for both water stage and constituents. These compartments are generally located towards the northern and the western sides of the canal and the north western marsh of the Refuge. For those compartments in the canal, the good agreement is attributed to the impact of the inflow boundary. Three approaches, namely ASC, ISC, and MAC were used for the comparison. Although a series of statistical measures were calculated and considered, bias, average of observed and simulated, standard deviation of observed and simulated and NSE were of more emphasis. In big interior marsh compartments, the 39-Compartment Model prediction uses one value to represent the whole compartment, but the Spatially Explicit Model uses much higher resolution grid, thus better captures concentration variation within that compartment. Shrestha (2011) concluded that the bathymetry of the marsh compartments 20 and 22 of the 39-compartment model is inaccurate. The bathymetry has been revised before this comparison based on the bathymetry of the Spatially Explicit Model.

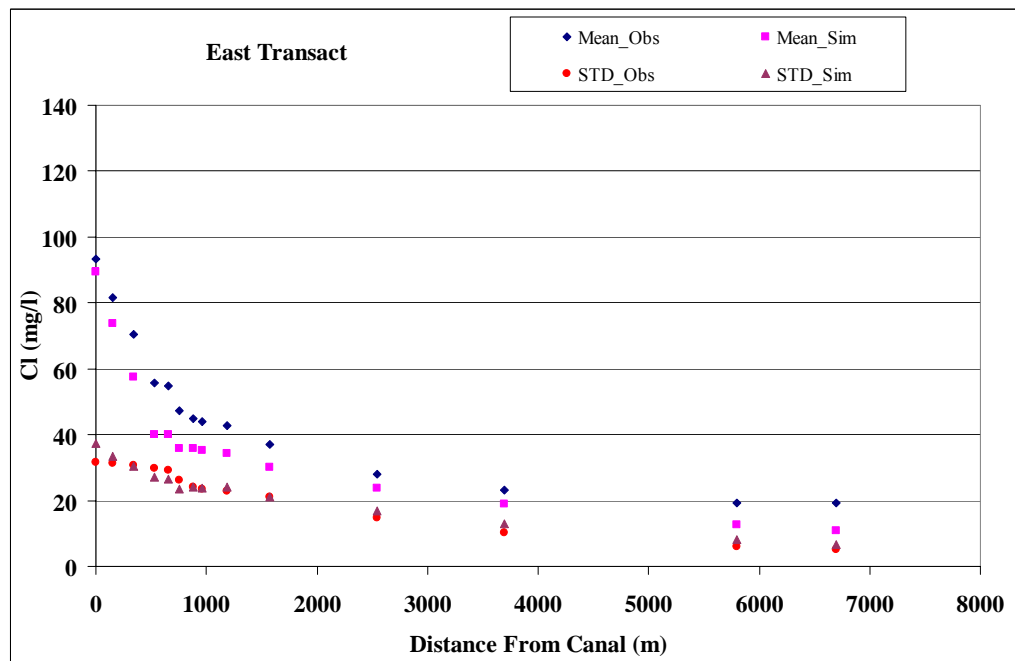


Figure 13 – 3-point moving average of mean and standard deviation of modeled and observed for the Spatially Explicit Model on the east transect

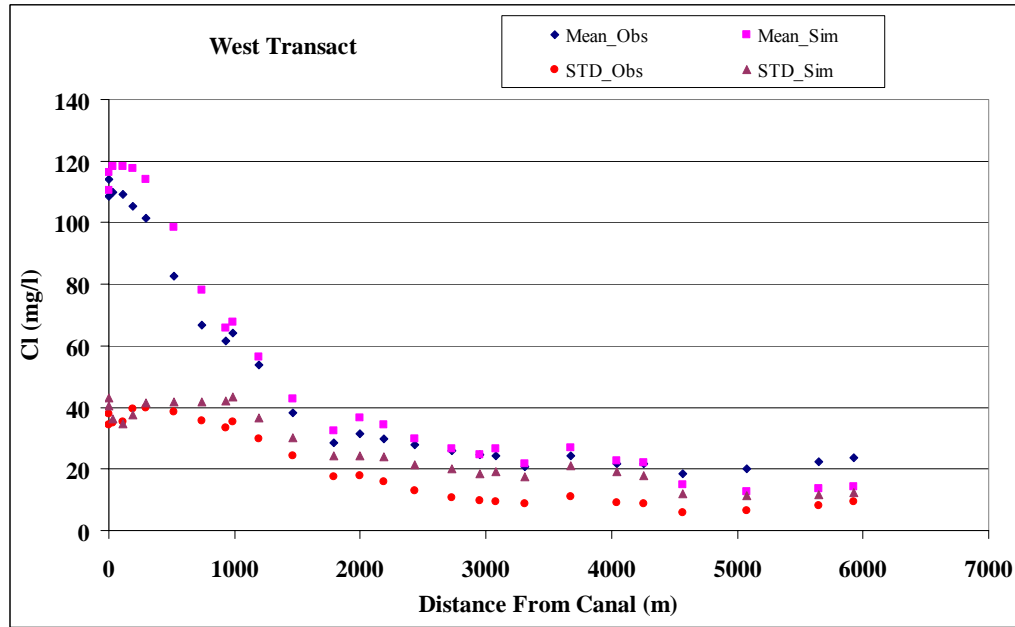


Figure 14 – 3-point moving average of mean and standard deviation of modeled and observed for the Spatially Explicit Model on the west transect

9.5 Conclusions

In this chapter, two models - the 39-Compartment Model based on Berkeley Madonna and the Spatially Explicit Model based on MIKE FLOOD (DHI) that were developed for modeling the water and chloride transport in the Refuge were compared using observed data. Model comparison with observed data using different techniques not only helped us to evaluate each of these models credibility, but also helped us to find which of the comparison techniques can be used in the future to get better statistical results for research investigations, management applications, and prediction purposes. There would be limitations, uncertainties or problems in each of these methods, where comparison with observed data confirms which are useful for future improvements of each model. It is concluded that NSE cannot be the only statistical tool to evaluate each model, but bias, average of observed and simulated values, standard deviation of observed and simulated values are also some influential

statistical tools in model evaluation. It is also concluded that the Spatially Explicit Model, can provide more accurate prediction to the observed data for the Refuge in general, by having the best approaches in three out of four type compartments (canal, peripheral marsh, transitional marsh, and interior marsh).

The 39-Compartment Model results represent spatially aggregated (11 canal and 28 marsh compartments) canal and marsh values for all state variables (e.g., volume, stage, and water quality parameters). The 39-Compartment Model can be used to detect water quality variations along western and eastern gradients as well as north-to-south gradient. Due to its spatially aggregated nature, the model is not desired to be used to analyze site specific events. The Spatially Explicit Model results provide detailed spatial and temporal information of hydrodynamic and water quality state variables. This model can be used to analyze site specific events. Depending on the time scale of input data, Mike Flood can be used for analyzing short term (transient) to long term (daily, monthly or annual) events. In view of its computational cost, it is feasible to run decadal simulation within reasonable amount of time.

Appendix A

Statistics for water stage, chloride, sulfate, and total phosphorus for compartments in the Refuge with available observing sites

Compartment	Bias(m)	Ave Obs.(m)	Ave Sim(m)	RMSE(m)	SID Obs.(m)	SID Sim(m)	SID Error(m)	Variance Reduction	R(Correl Coef)	R ²	NSE
C2	0.04	4.92	4.96	0.13	0.27	0.25	0.12	80%	0.89	0.80	0.77
C3	0.05	4.92	4.97	0.13	0.26	0.25	0.12	79%	0.89	0.79	0.75
C4	0.09	4.91	5.00	0.16	0.28	0.23	0.13	80%	0.90	0.80	0.69
C5	0.02	4.90	4.92	0.12	0.25	0.24	0.12	76%	0.88	0.77	0.76
C6	-0.02	4.97	4.94	0.14	0.23	0.23	0.14	63%	0.81	0.66	0.62
C7	0.05	4.88	4.93	0.16	0.27	0.24	0.15	67%	0.82	0.67	0.63
C8	0.01	4.92	4.94	0.16	0.25	0.23	0.15	62%	0.83	0.68	0.64
C9	-0.01	4.95	4.94	0.12	0.26	0.23	0.12	77%	0.88	0.77	0.77
C11	0.06	4.89	4.96	0.16	0.27	0.24	0.14	71%	0.85	0.72	0.66
M5	-0.02	5.06	5.03	0.07	0.12	0.11	0.06	71%	0.85	0.73	0.67
M7	0.04	4.98	5.02	0.10	0.17	0.14	0.09	72%	0.85	0.72	0.67
M8	0.00	4.93	4.93	0.07	0.20	0.20	0.07	86%	0.93	0.87	0.86

Table 8 – Statistics of water level for canal and marsh compartments with available observing sites for 1/1/1998 to 12/31/2010

Compartment	Bias(mg/l)	Mean_Obs(mg/l)	Mean_Sim(mg/l)	RMSE(mg/l)	SD_Obs(mg/l)	SD_Sim(mg/l)	SD_Error(mg/l)	Variance Reduction	R(Correl Coef)	R^2	NSE
C3	-10.20	110.25	100.05	25.73	36.51	36.59	23.78	58%	0.79	0.62	0.50
C4	-7.35	118.47	111.12	27.39	39.36	34.21	26.41	55%	0.75	0.56	0.51
C5	-5.47	108.91	103.44	23.67	37.65	35.61	23.10	62%	0.80	0.64	0.60
C6	-3.15	91.16	88.01	27.20	37.63	33.66	27.16	48%	0.72	0.51	0.47
C7	2.88	78.56	81.43	29.28	33.96	30.16	29.29	26%	0.59	0.35	0.25
C8	-6.34	82.86	76.52	27.06	33.41	27.68	26.38	38%	0.64	0.41	0.34
C9	6.08	74.23	80.31	24.86	29.57	28.80	24.21	33%	0.66	0.43	0.29
C10	-11.17	93.29	82.12	27.04	31.89	26.93	24.68	40%	0.66	0.44	0.28
M17	-24.98	79.98	55.00	45.48	37.44	28.27	38.42	-5%	0.34	0.12	-0.51
M18	-25.42	112.43	87.01	37.80	35.00	29.90	28.04	36%	0.64	0.41	-0.17
M19	-8.19	79.41	70.45	28.68	41.16	31.54	27.53	55%	0.77	0.59	0.53
M23	1.98	55.88	57.87	33.15	32.29	29.09	33.21	-6%	0.42	0.18	-0.06
M27	10.09	25.98	35.88	30.79	18.24	24.17	29.20	-156%	0.07	0.01	-1.85
M28	-11.37	43.96	32.59	30.52	25.67	23.66	28.40	-22%	0.34	0.12	-0.42
M30	-8.36	55.99	47.63	23.16	30.42	19.97	21.67	49%	0.70	0.49	0.42
M31	-4.56	47.56	43.00	23.55	28.03	20.72	23.13	32%	0.59	0.34	0.29
M33	-17.79	62.18	44.38	41.24	35.07	22.38	37.39	-14%	0.21	0.04	-0.40
M34	-5.98	35.09	29.11	26.44	22.24	18.14	25.80	-35%	0.20	0.04	-0.42
M35	6.25	21.92	28.17	24.37	11.93	20.81	23.61	-292%	0.04	0.00	-3.19
M36	4.07	37.50	41.51	28.30	31.54	29.06	28.02	21%	0.58	0.33	0.19
M37	-3.84	25.19	21.31	22.30	15.53	16.56	21.98	-100%	0.07	0.00	-1.06
M38	20.40	31.04	51.44	37.28	23.34	29.40	31.26	-79%	0.31	0.10	-1.56
M39	2.56	23.56	26.12	26.63	14.49	20.37	26.55	-236%	-0.14	0.02	-2.39

Table 9 – Statistics of chloride concentration for canal and marsh compartments with available observing sites for 1/1/1998 to 12/31/2010

Compartment	Bias(mg/l)	Mean_Obs(mg/l)	Mean_Sim(mg/l)	RMSE(mg/l)	SD_Obs(mg/l)	SD_Sim(mg/l)	SD_Error(mg/l)	Variance Reduction	R(Correl Coef)	R^2	NSE
C3	-1.00	44.89	43.88	13.06	23.85	23.78	13.11	70%	0.85	0.72	0.70
C4	-7.54	50.75	43.21	16.96	22.62	21.04	15.21	55%	0.76	0.58	0.44
C5	-6.12	49.96	43.84	14.68	24.92	23.12	13.44	71%	0.85	0.72	0.65
C6	-3.77	40.33	36.01	17.32	23.33	21.42	17.02	47%	0.79	0.62	0.46
C7	-0.03	30.20	30.18	13.96	18.90	18.52	14.06	45%	0.72	0.52	0.45
C8	-7.64	30.23	22.59	15.49	19.05	15.32	13.55	49%	0.71	0.50	0.33
C9	-1.71	26.33	24.62	15.07	19.20	13.93	15.12	38%	0.62	0.39	0.37
C10	-6.10	29.13	29.13	17.48	20.01	13.26	16.42	33%	0.58	0.33	0.23
M17	-1.55	19.12	17.57	13.18	17.96	16.79	13.23	46%	0.71	0.51	0.45
M18	-19.98	46.79	26.81	26.95	22.13	16.50	18.13	33%	0.59	0.35	-0.49
M19	-3.68	24.05	20.38	16.74	20.69	14.56	16.36	37%	0.62	0.38	0.34
M23	-5.16	15.39	10.23	16.66	16.64	10.07	15.90	9%	0.37	0.14	-0.01
M27	1.54	2.76	4.31	8.95	6.33	8.45	8.85	-96%	0.31	0.10	-1.02
M28	-1.30	6.27	4.98	11.58	11.53	9.37	11.54	0%	0.41	0.16	-0.01
M30	0.06	8.28	8.28	6.87	12.23	9.37	6.89	68%	0.83	0.68	0.68
M31	0.35	6.81	7.16	9.17	11.81	8.46	9.17	40%	0.64	0.40	0.40
M33	-1.77	8.85	7.08	12.23	11.87	8.66	12.16	-5%	0.33	0.11	-0.07
M34	-0.26	5.04	4.77	10.05	10.03	8.40	10.06	-1%	0.42	0.17	-0.01
M35	2.28	0.94	3.22	6.84	3.53	5.85	6.46	-236%	0.12	0.01	-2.78
M36	-0.19	5.61	5.26	19.76	20.10	7.46	19.77	3%	0.20	0.04	0.01
M37	-1.02	1.60	0.58	6.59	6.44	1.32	6.52	-3%	0.04	0.00	-0.05
M38	4.93	2.83	7.76	10.70	6.72	9.46	9.51	-101%	0.35	0.12	-1.55
M39	-0.59	1.52	0.93	4.77	4.44	2.34	4.74	-14%	0.13	0.02	-0.15

Table 10 – Statistics of sulfate concentration for canal and marsh compartments with available observing sites for 1/1/1998 to 12/31/2010

Compartment	Bias(µg/l)	Mean_Obs(µg/l)	Mean_Sim(µg/l)	RMSE(µg/l)	SD_Obs(µg/l)	SD_Sim(µg/l)	SD_Error(µg/l)	Variance Reduction	R(Correl Coef)	R^2	NSE
C3	-5.88	58.32	52.45	20.19	45.68	44.98	19.45	82%	0.91	0.82	0.80
C4	12.28	47.12	59.40	28.55	36.73	38.99	25.81	51%	0.77	0.59	0.39
C5	-6.53	54.69	48.16	37.22	49.22	36.60	36.75	44%	0.67	0.45	0.42
C6	1.54	35.33	36.87	31.96	32.06	27.02	32.09	0%	0.42	0.18	0.00
C7	2.41	31.53	33.94	19.01	26.96	24.13	18.95	51%	0.73	0.53	0.50
C8	4.98	30.54	35.52	19.58	20.17	27.85	18.98	11%	0.73	0.54	0.05
C9	-21.75	65.21	43.46	71.05	70.76	36.47	67.85	8%	0.34	0.11	-0.01
C10	2.77	68.27	45.00	52.61	74.86	42.24	47.29	60%	0.81	0.66	0.50
M17	0.64	21.94	14.40	25.27	32.79	10.06	24.37	45%	0.88	0.78	0.39
M18	1.43	32.63	27.79	37.88	30.46	22.19	37.63	-53%	0.00	0.00	-0.55
M19	0.22	11.05	16.90	14.70	7.82	9.74	13.51	-198%	-0.17	0.03	-2.54
M23	0.08	7.51	11.14	8.84	2.86	7.48	8.09	-700%	-0.03	0.00	-8.62
M27	0.02	7.89	9.88	4.40	2.81	4.59	3.94	-96%	0.52	0.27	-1.47
M28	0.09	8.30	11.84	9.61	4.34	8.73	8.96	-325%	0.20	0.04	-3.92
M30	1.94	32.73	15.82	44.04	47.80	13.74	40.80	27%	0.62	0.38	0.15
M31	-1.27	13.35	12.08	14.35	16.75	6.67	14.31	27%	0.54	0.29	0.26
M33	1.57	13.77	15.34	9.80	10.20	10.31	9.72	9%	0.55	0.30	0.07
M34	1.36	9.69	11.06	8.28	7.37	4.51	8.18	-23%	0.12	0.01	-0.27
M35	-0.27	9.46	9.18	5.26	4.78	2.96	5.27	-21%	0.14	0.02	-0.22
M36	0.72	8.13	8.84	8.26	8.26	3.57	8.26	0%	0.23	0.05	0.00
M37	-0.47	8.73	8.26	3.47	3.67	2.52	3.44	12%	0.43	0.19	0.11
M38	-0.26	8.55	8.29	4.53	3.95	3.37	4.53	-31%	0.24	0.06	-0.32
M39	-2.33	10.00	7.67	11.12	10.87	2.27	10.88	0%	0.10	0.01	-0.05

Table 11 – Statistics of total phosphorous concentration for canal and marsh compartments with available observing sites for 1/1/1998 to 12/31/2010

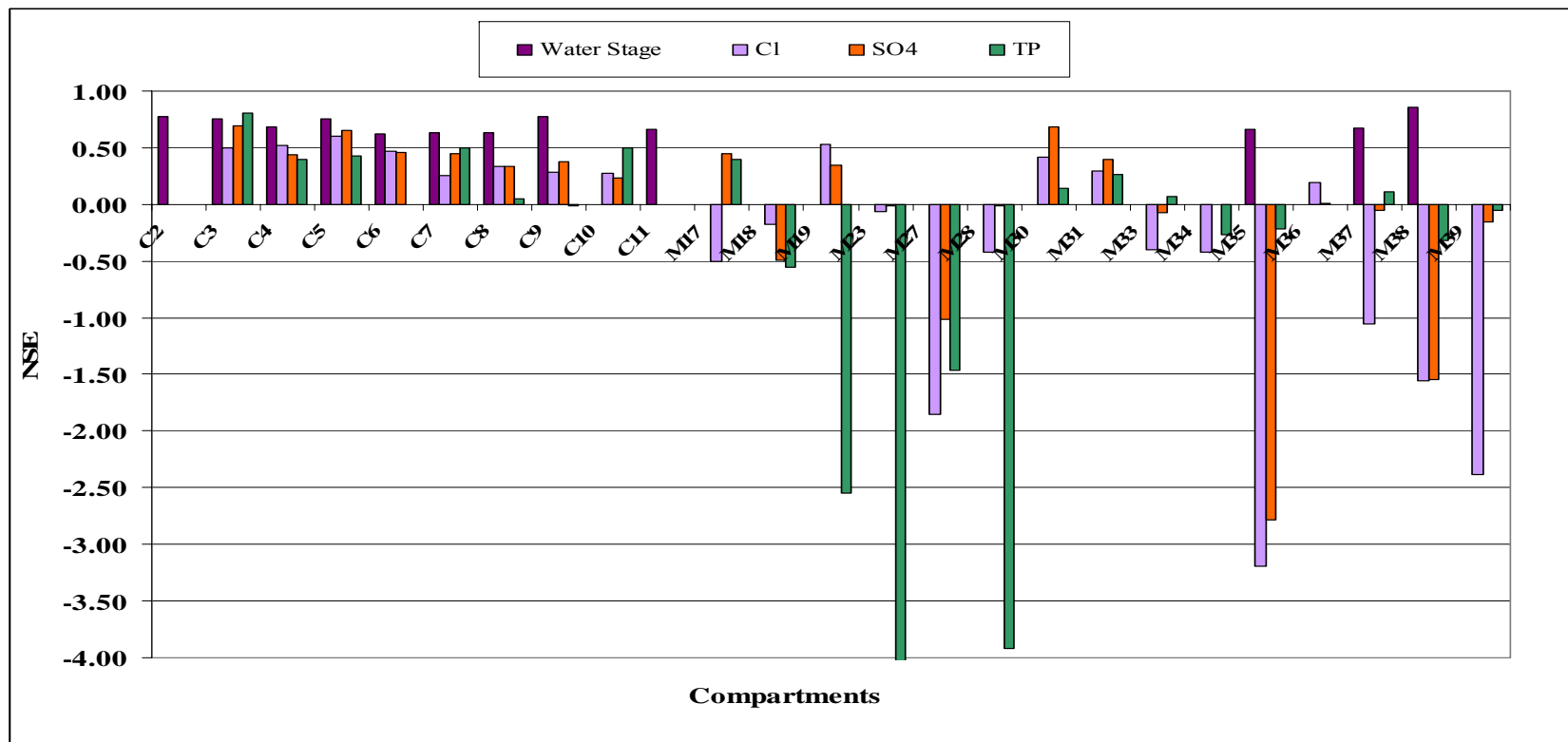


Figure 15 – Bar chart of Nash Sutcliff Efficiency for water stage, chloride, sulfate, total phosphorus concentrations in canal and marsh compartments for 1/1/1998 to 12/31/2010

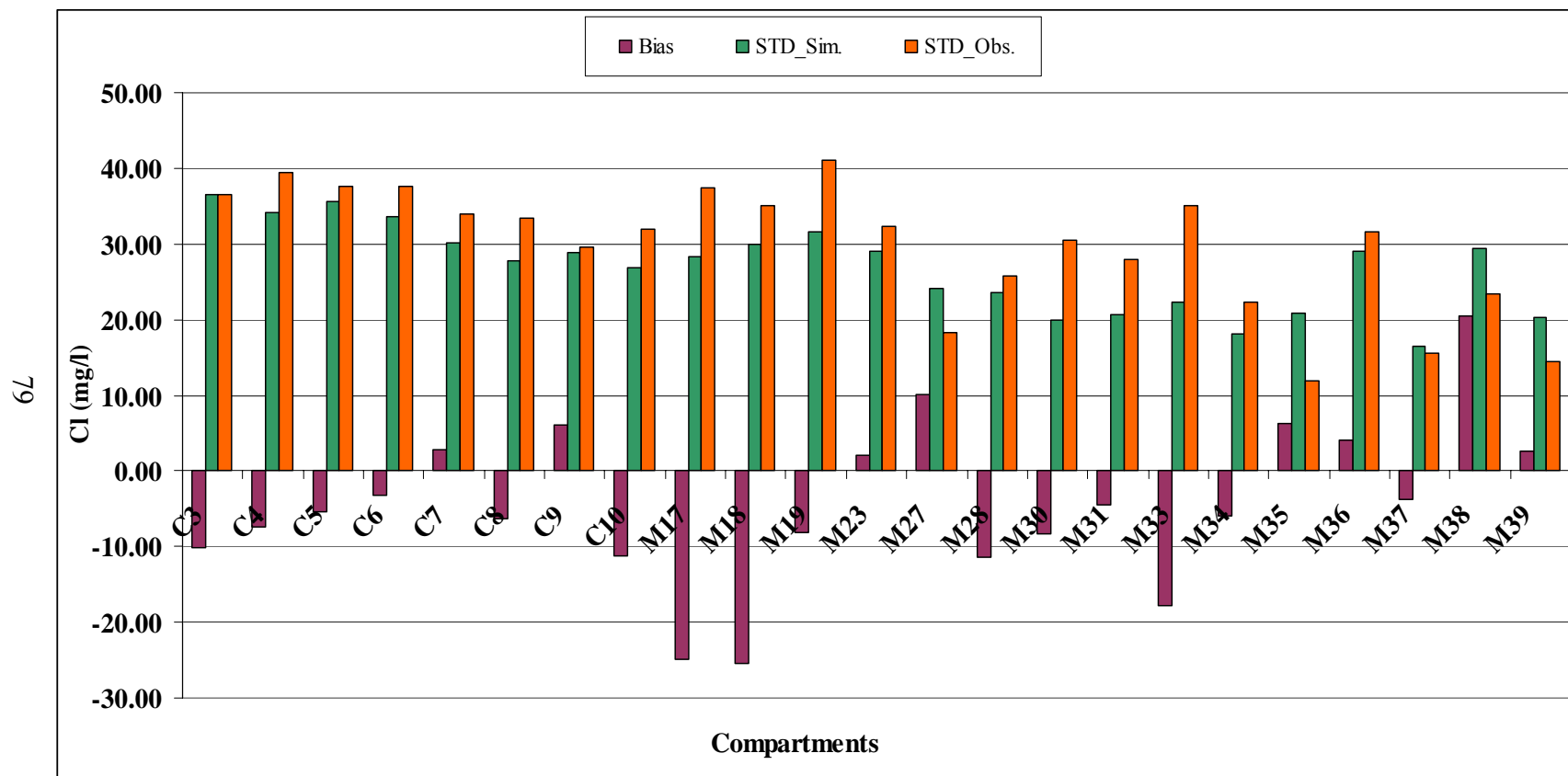


Figure 16 – Bar chart of bias, standard deviation of simulated and observed chloride concentration for the canal and marsh compartments for 1/1/1998 to 12/31/2010

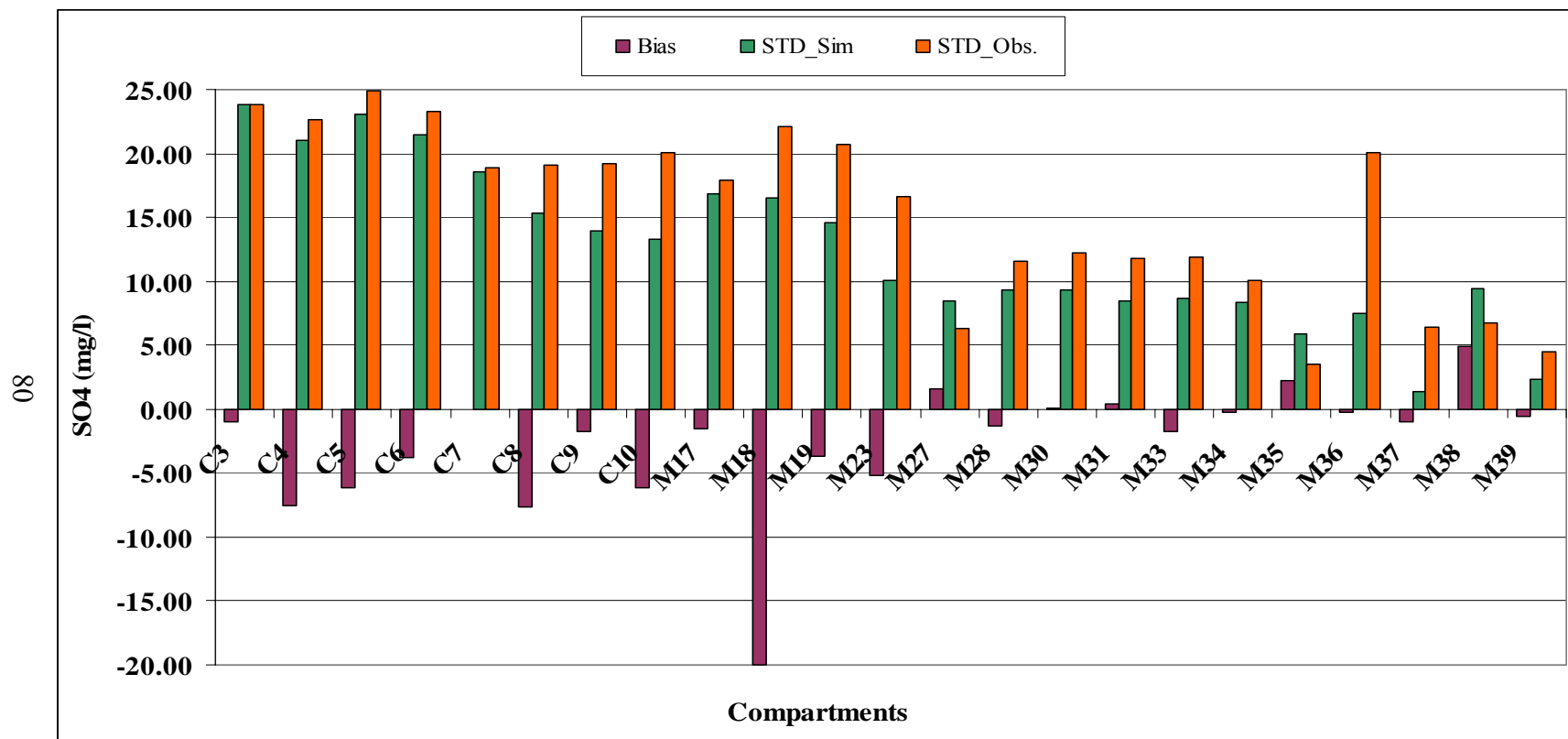


Figure 17 – Bar chart of bias, standard deviation of simulated and observed sulfate concentration for the canal and marsh compartments for 1/1/1998 to 12/31/2010

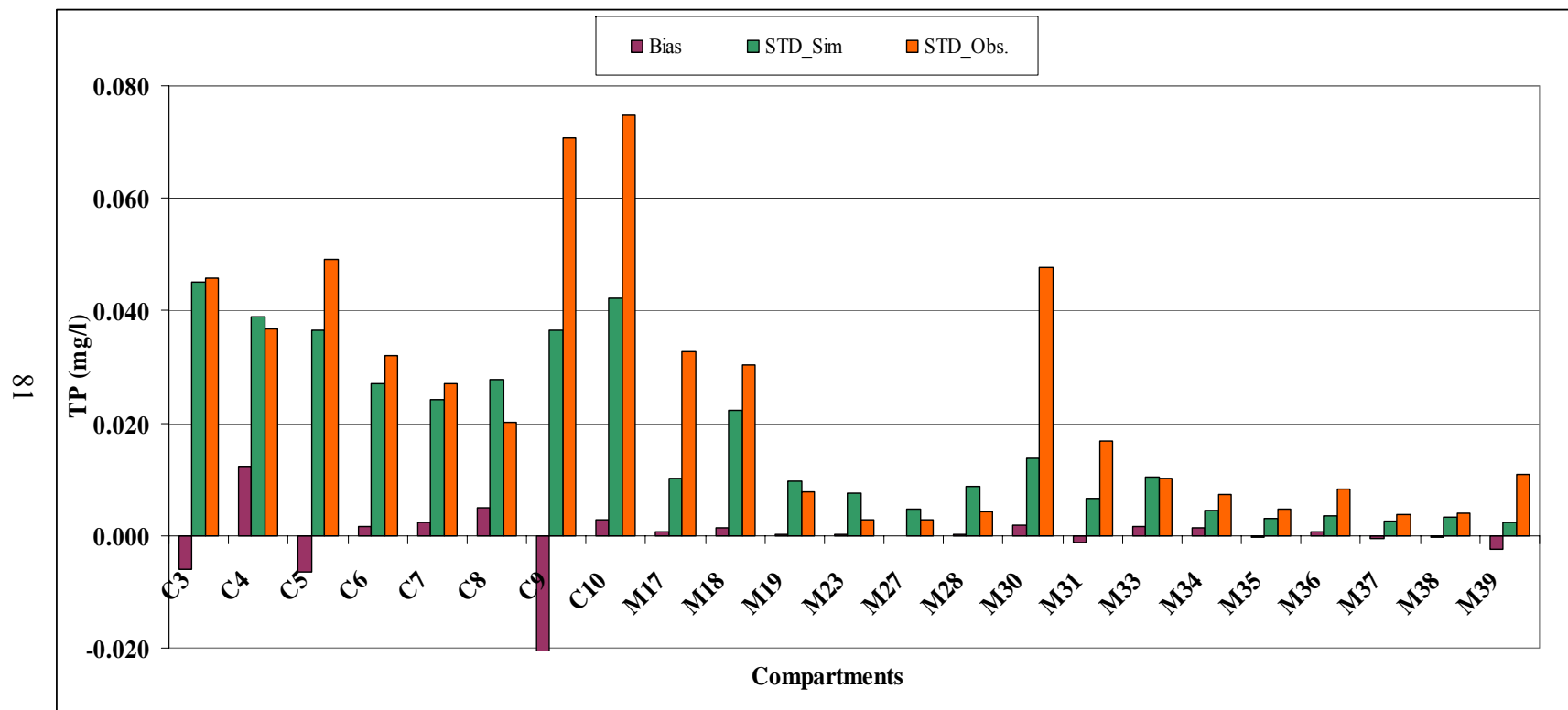


Figure 18 – Bar chart of bias, standard deviation of simulated and observed total phosphorous concentration for the canal and marsh compartments for 1/1/1998 to 12/31/2010

Appendix B

Comparison of simulated water stage with observed data within compartments

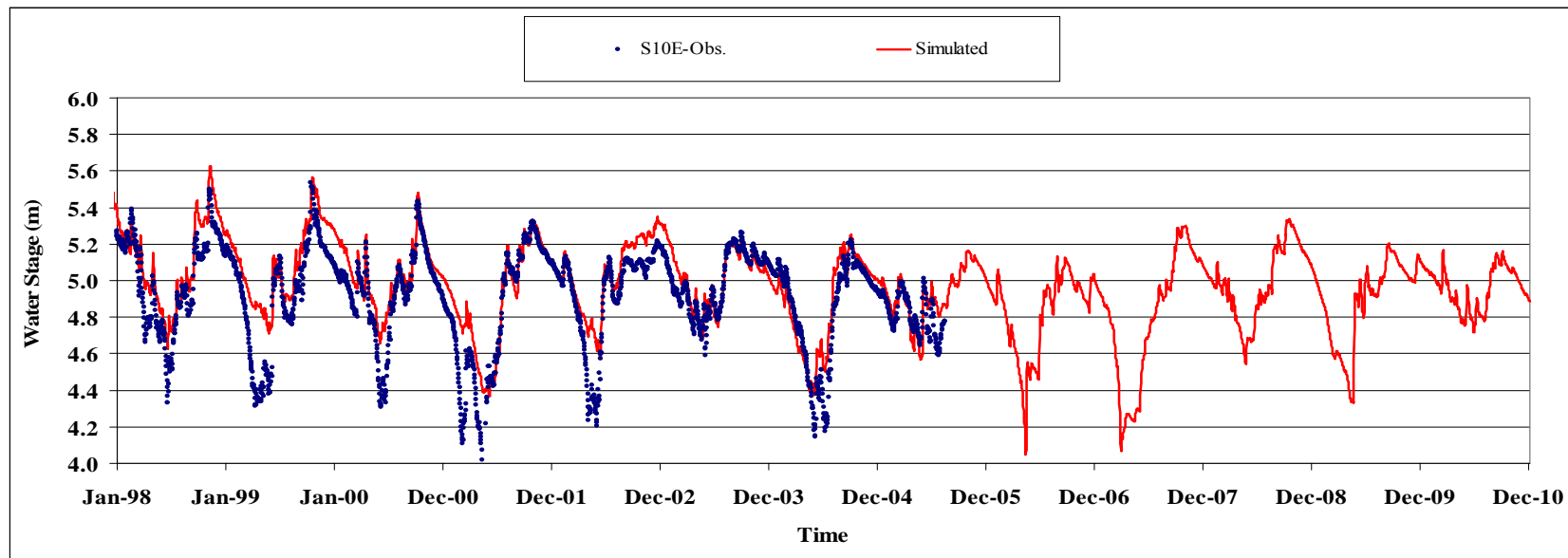


Figure 19 – Comparison of simulated water stage of C4 with observed data at stations within C4

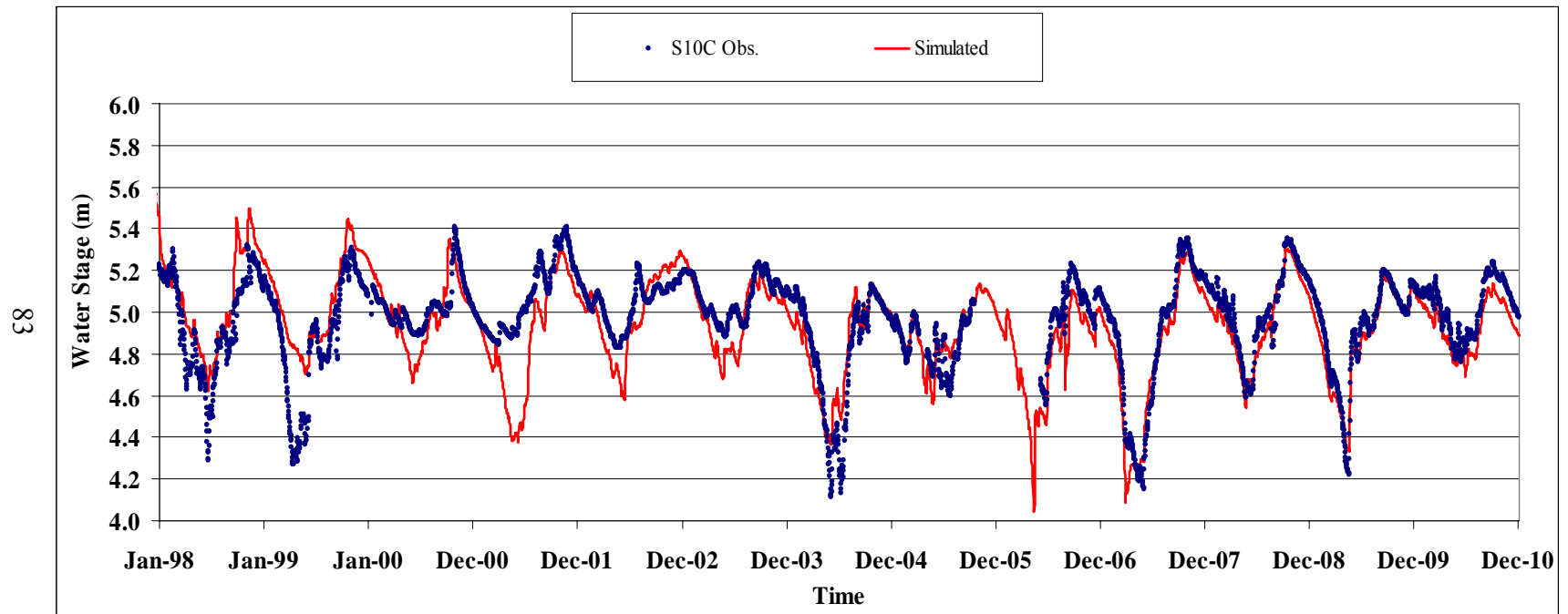


Figure 20 – Comparison of simulated water level of C6 with observed data at stations within C6

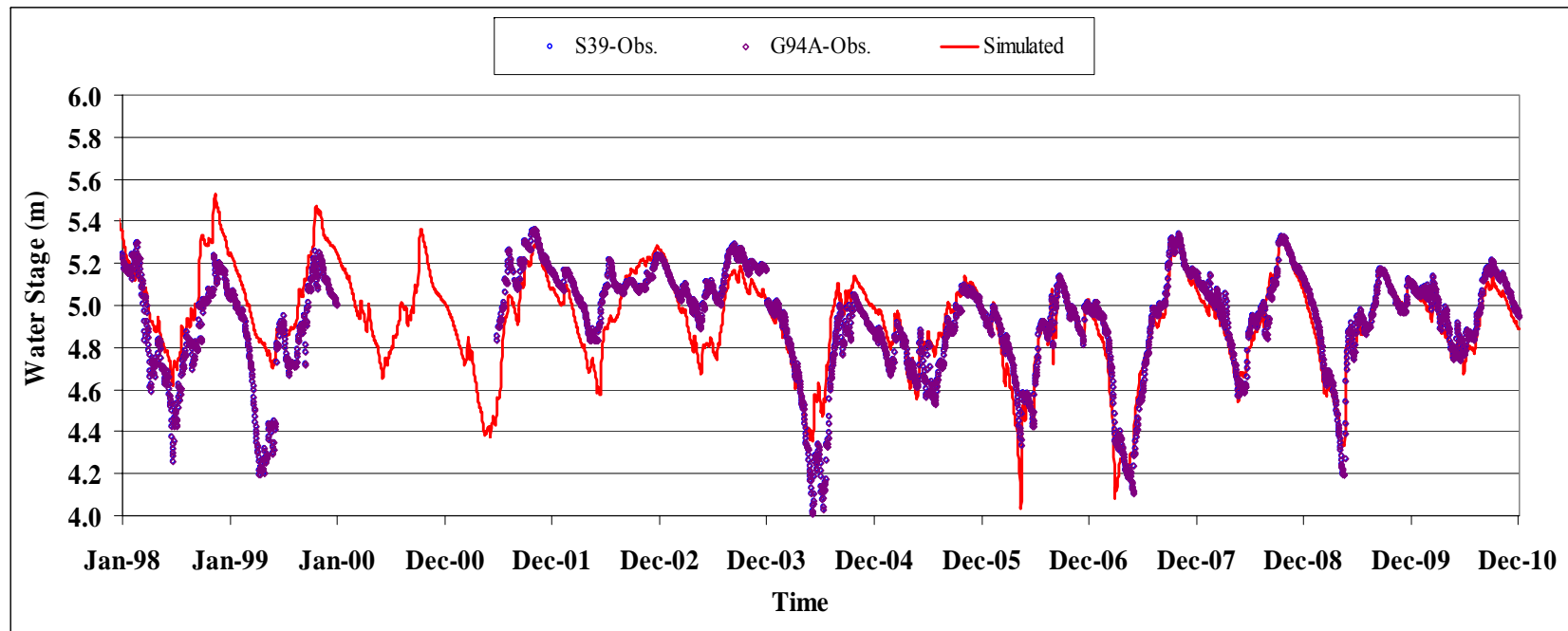


Figure 21 – Comparison of simulated water level of C8 with observed data at stations within C8

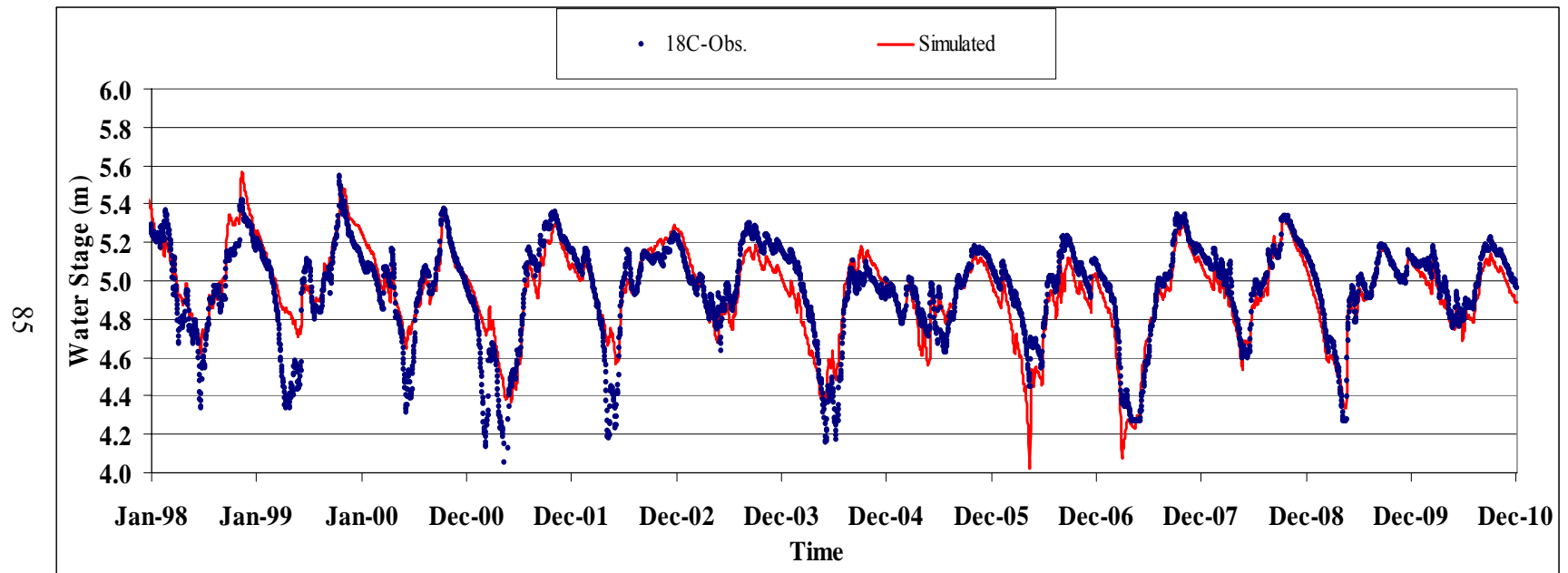


Figure 22 – Comparison of simulated water level of C9 with observed data at stations within C9

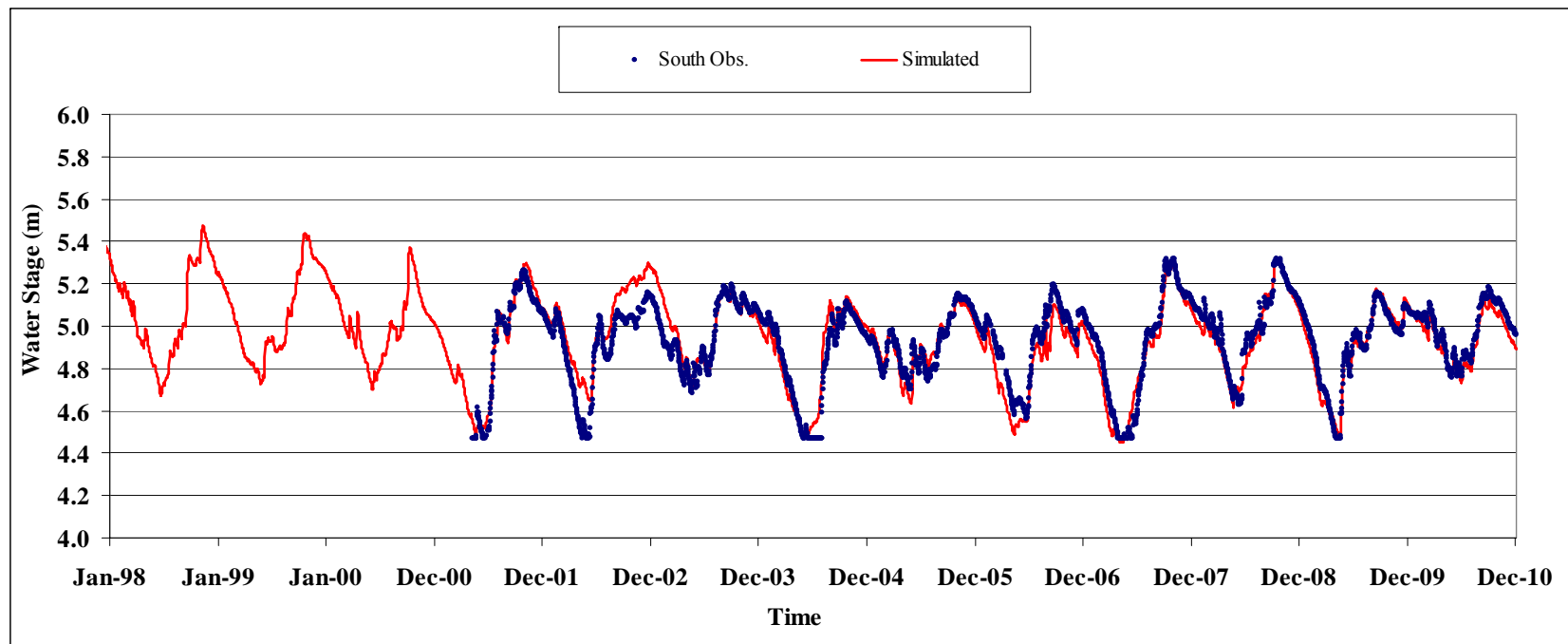


Figure 23 – Comparison of simulated water level of M38 with observed data at stations within M38

Appendix C

Comparison of simulated chloride concentration with observed data within compartments

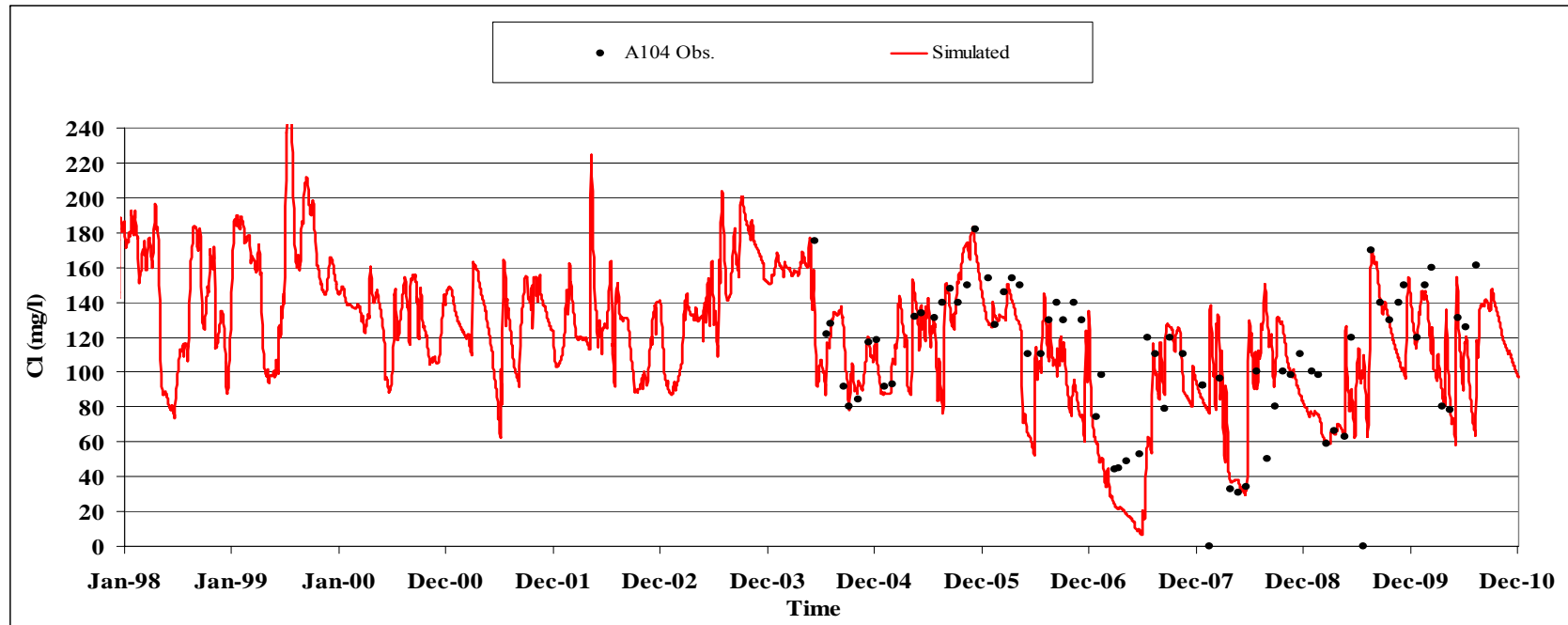


Figure 24 – Comparison of simulated chloride concentration of C3 with observed data at stations within C3

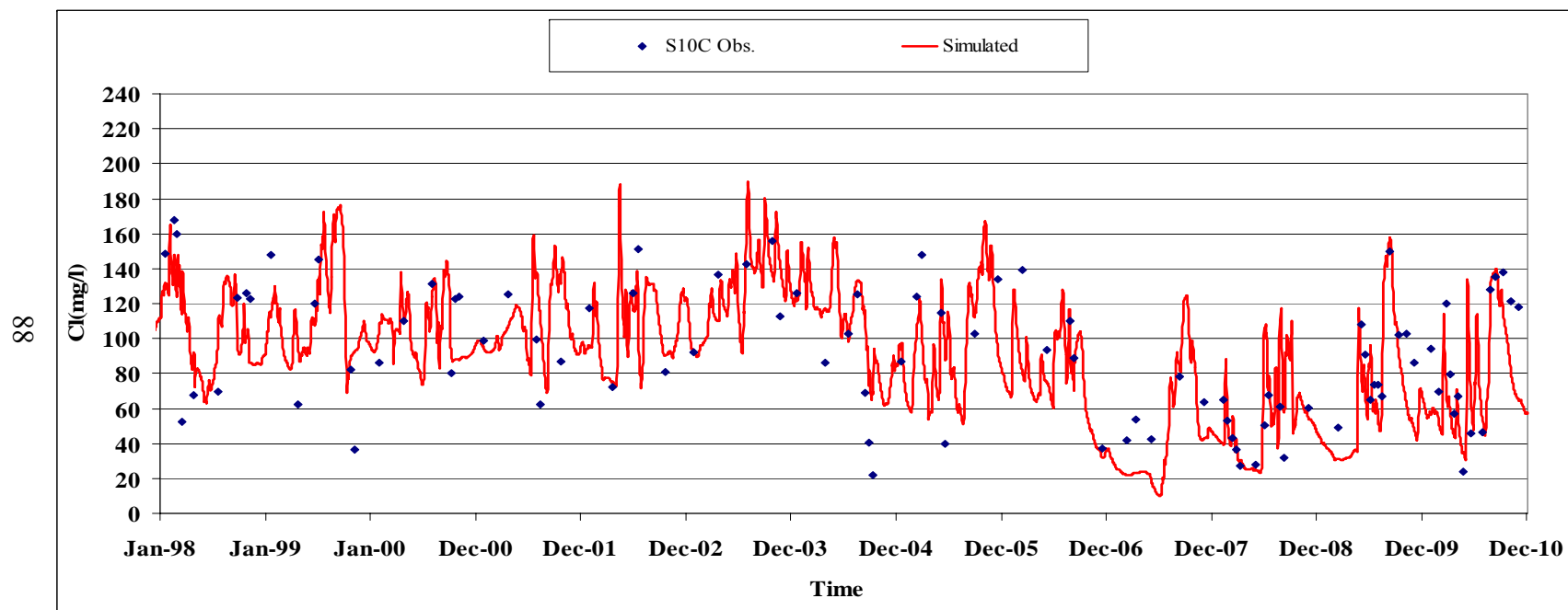


Figure 25 – Comparison of simulated chloride concentration of C6 with observed data at stations within C

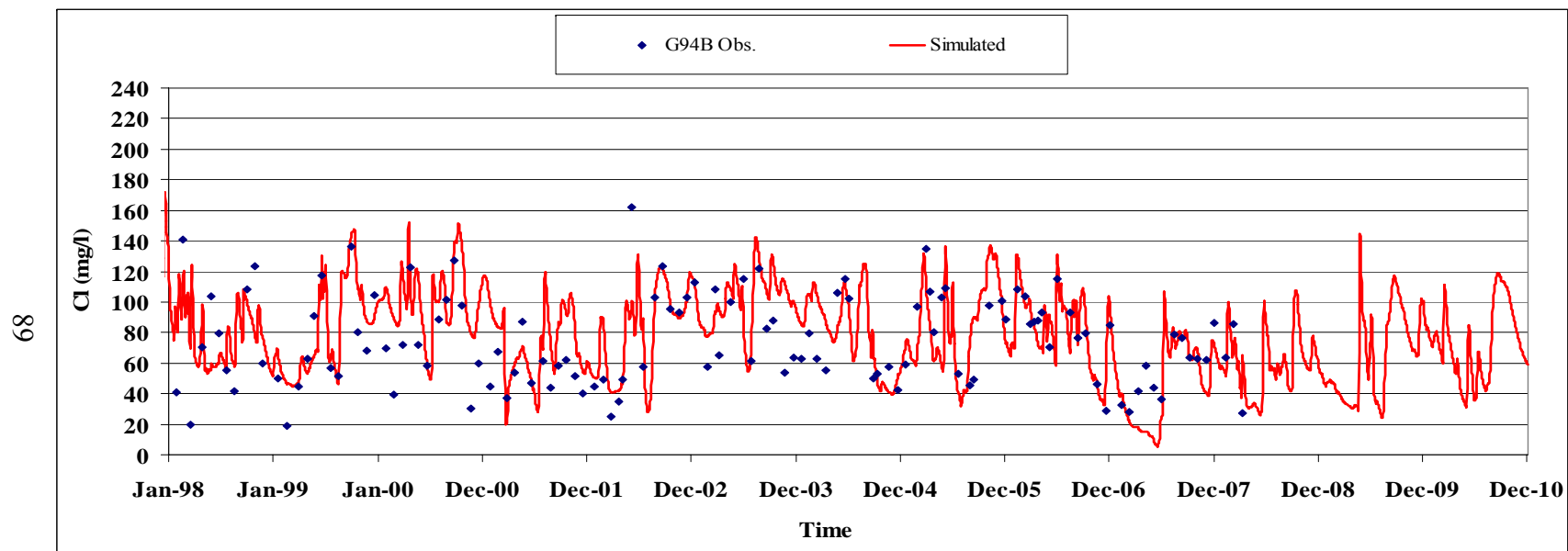


Figure 26 – Comparison of simulated chloride concentration of C9 with observed data at stations within C9

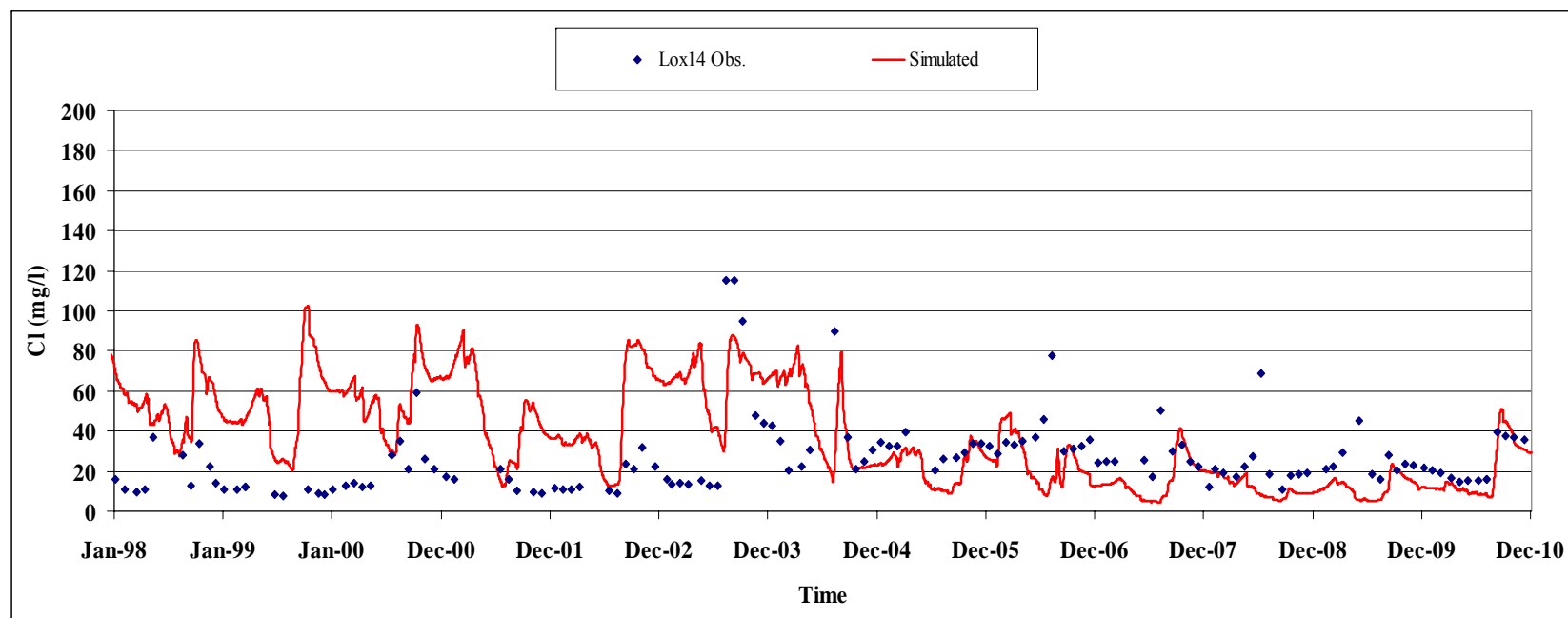


Figure 27 – Comparison of simulated chloride concentration of M27 with observed data at stations within M27

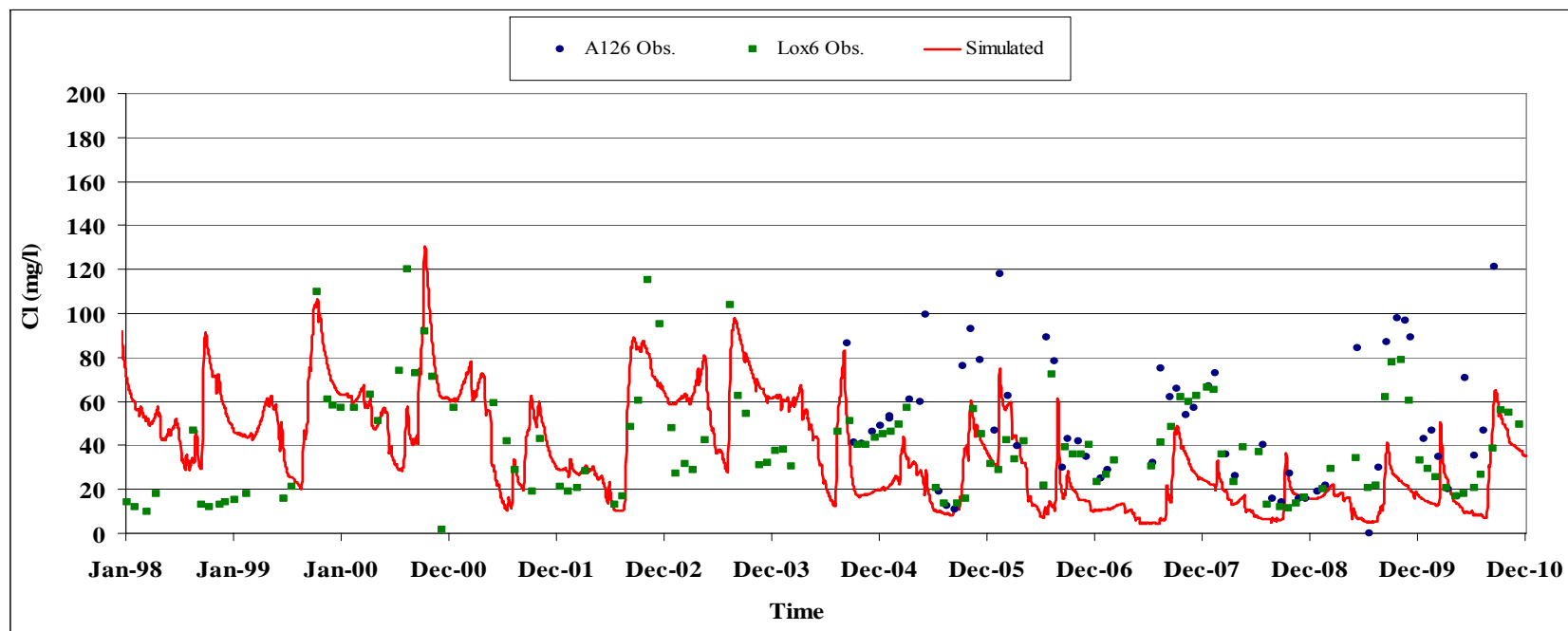


Figure 28 – Comparison of simulated chloride concentration of M28 with observed data at stations within M28

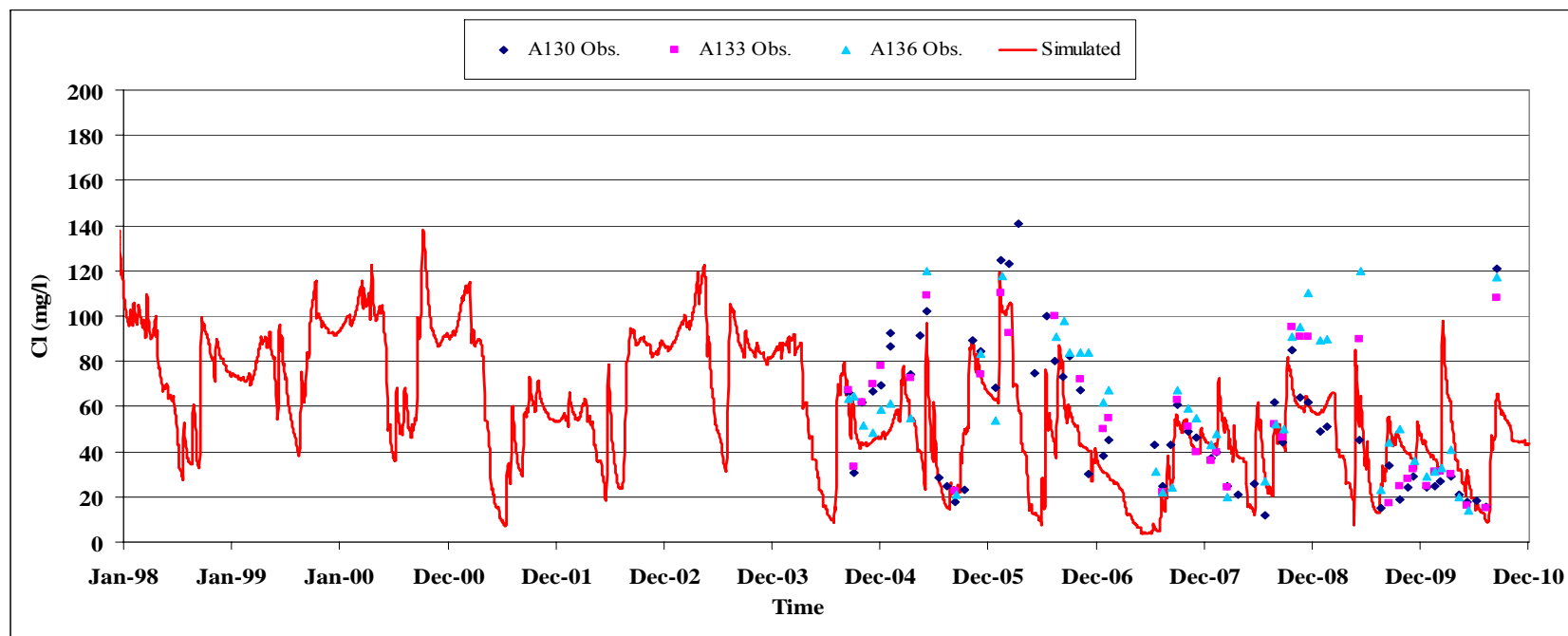


Figure 29 – Comparison of simulated chloride concentration of M30 with observed data at stations within M30

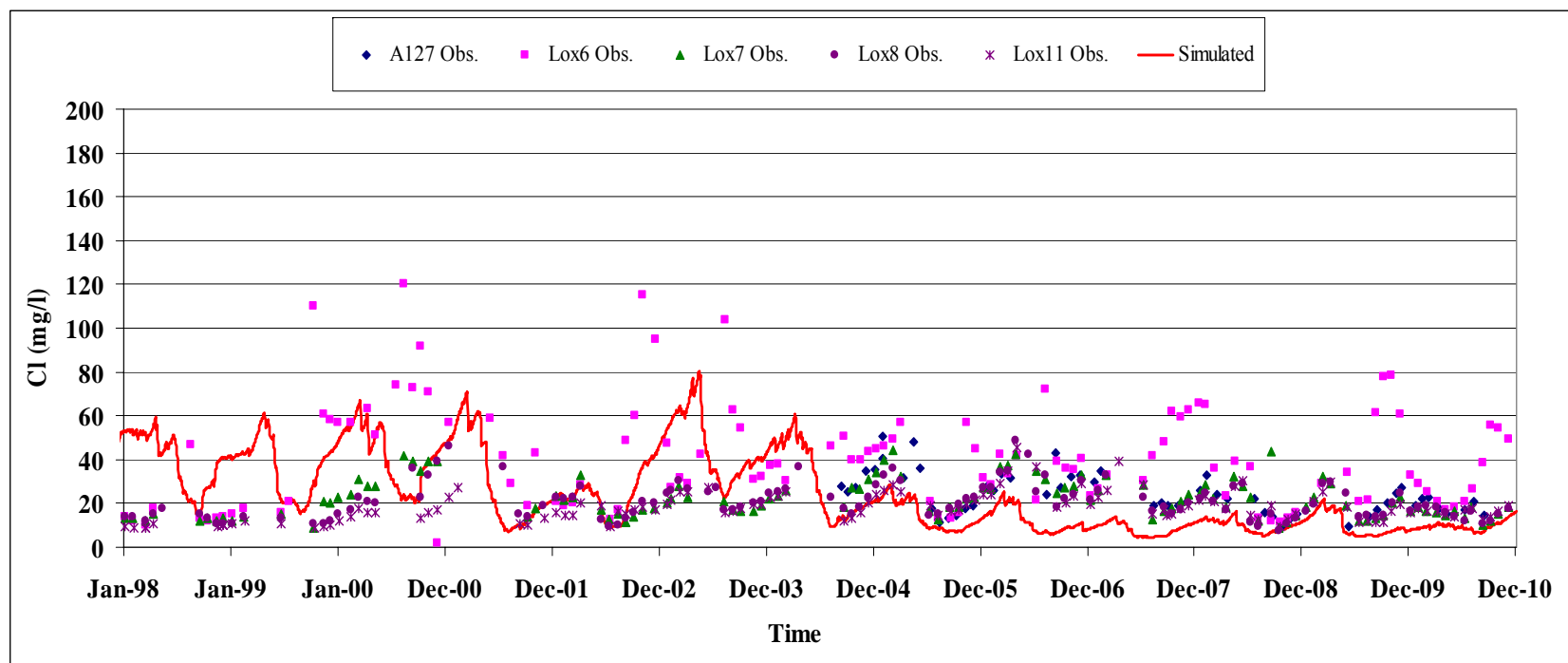


Figure 30 – Comparison of simulated chloride concentration of M37 with observed data at stations within M37

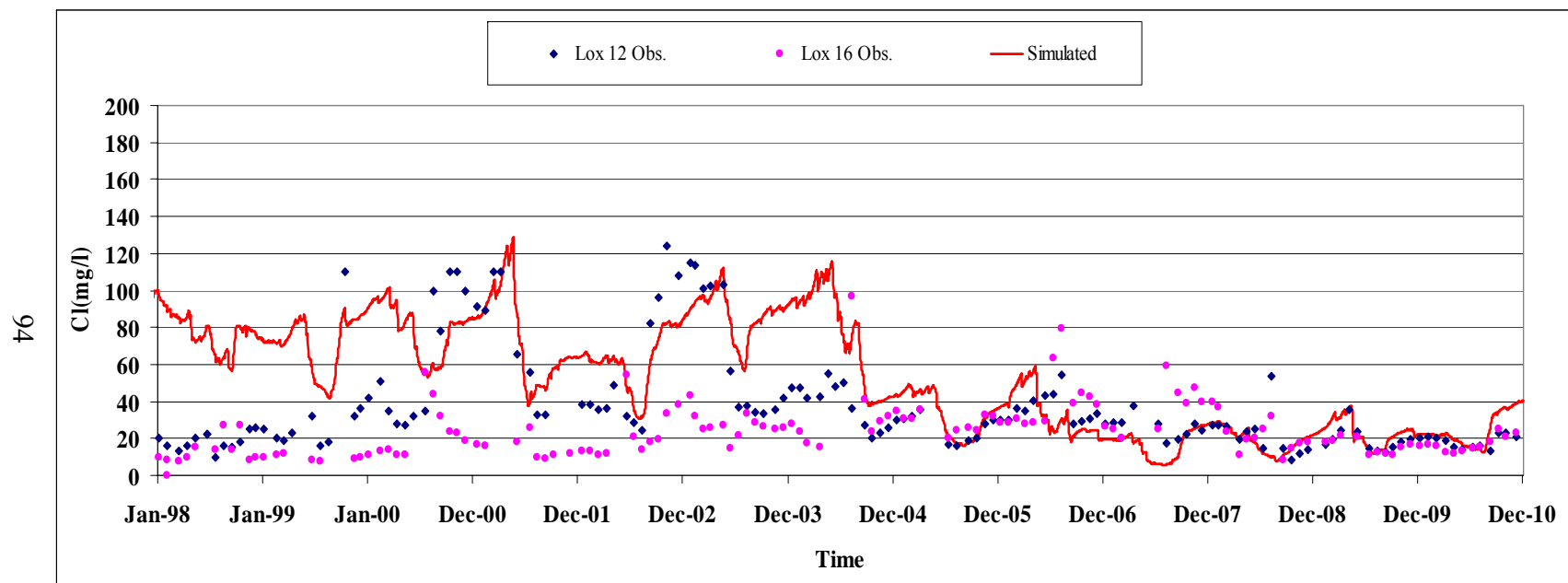


Figure 31 – Comparison of simulated chloride concentration of M38 with observed data at stations within M38

Appendix D

Comparison of simulated sulfate concentration with observed data within compartments

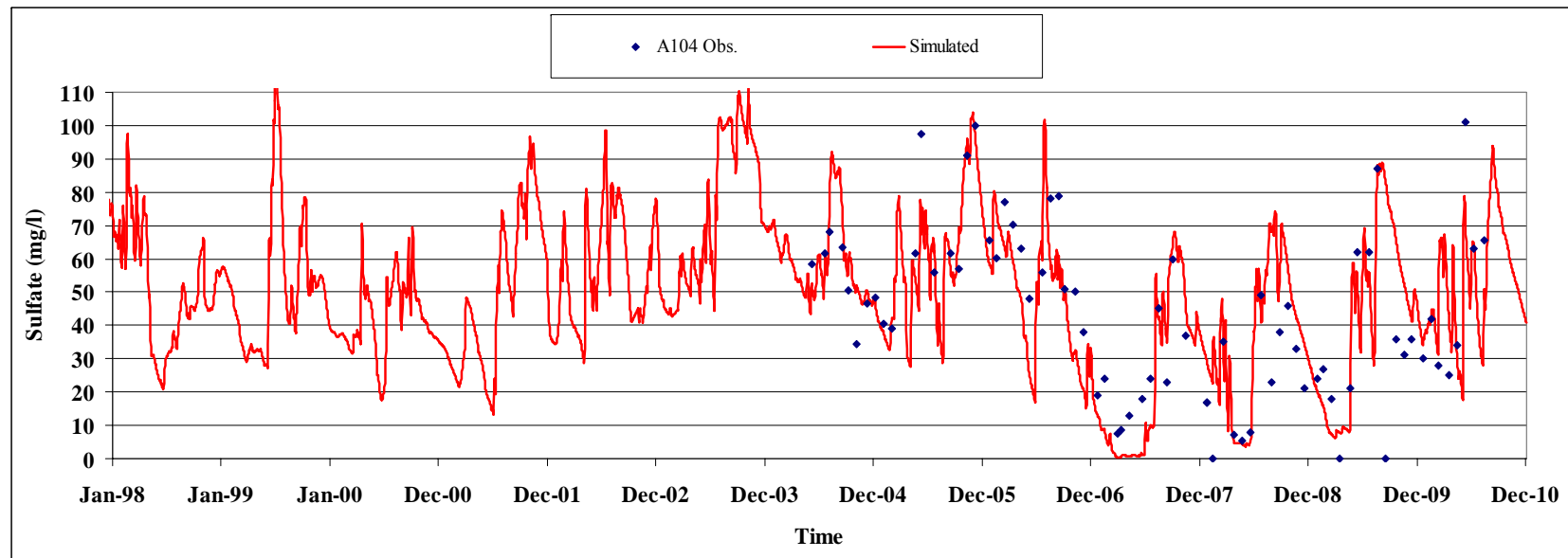


Figure 32 – Comparison of simulated sulfate concentration of C3 with observed data at stations within C3

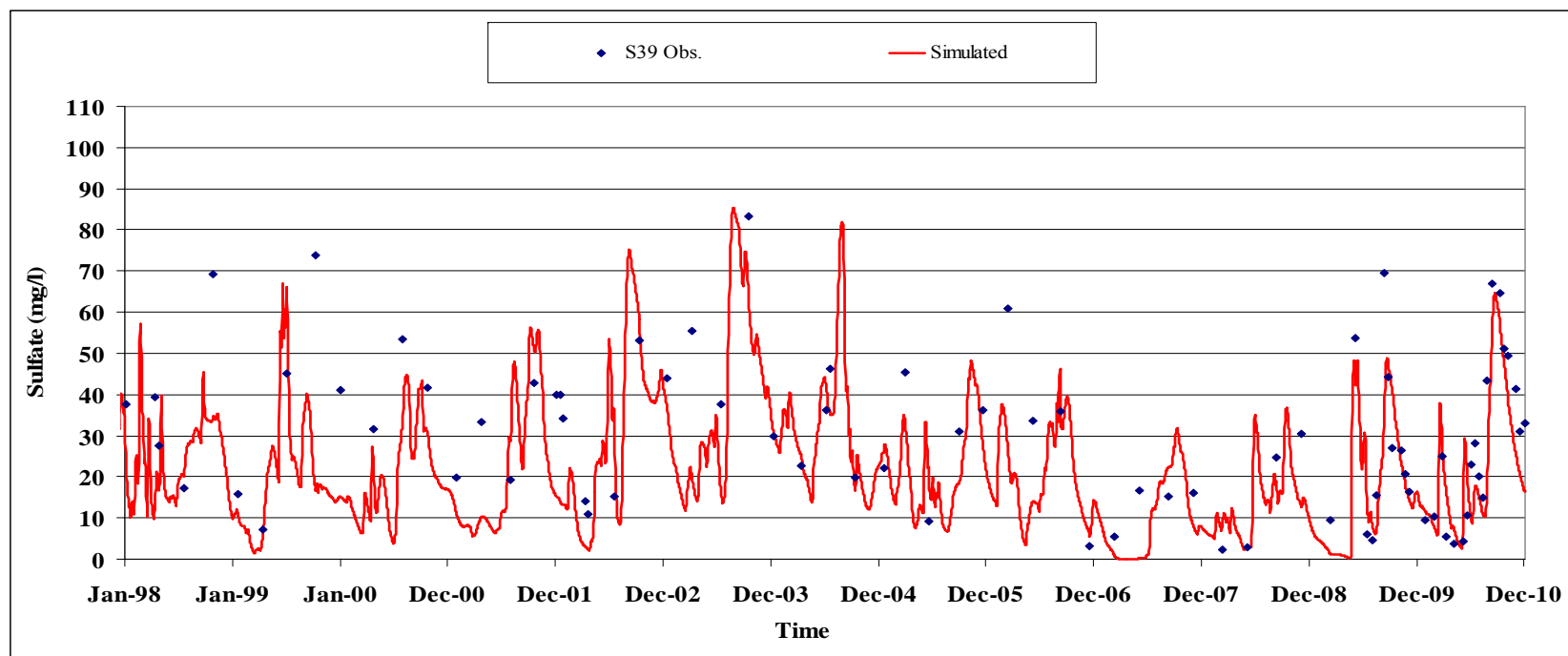


Figure 33 – Comparison of simulated sulfate concentration of C8 with observed data at stations within C8

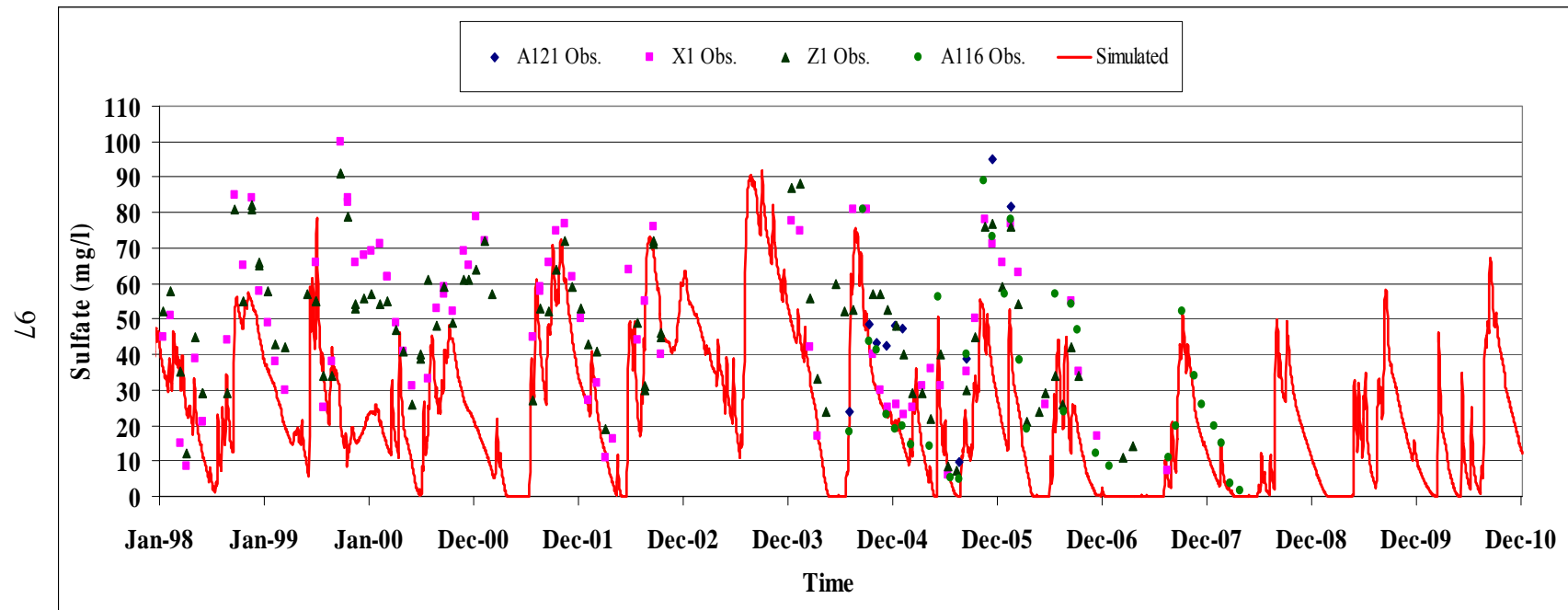


Figure 34 – Comparison of simulated sulfate concentration of M18 with observed data at stations within M18

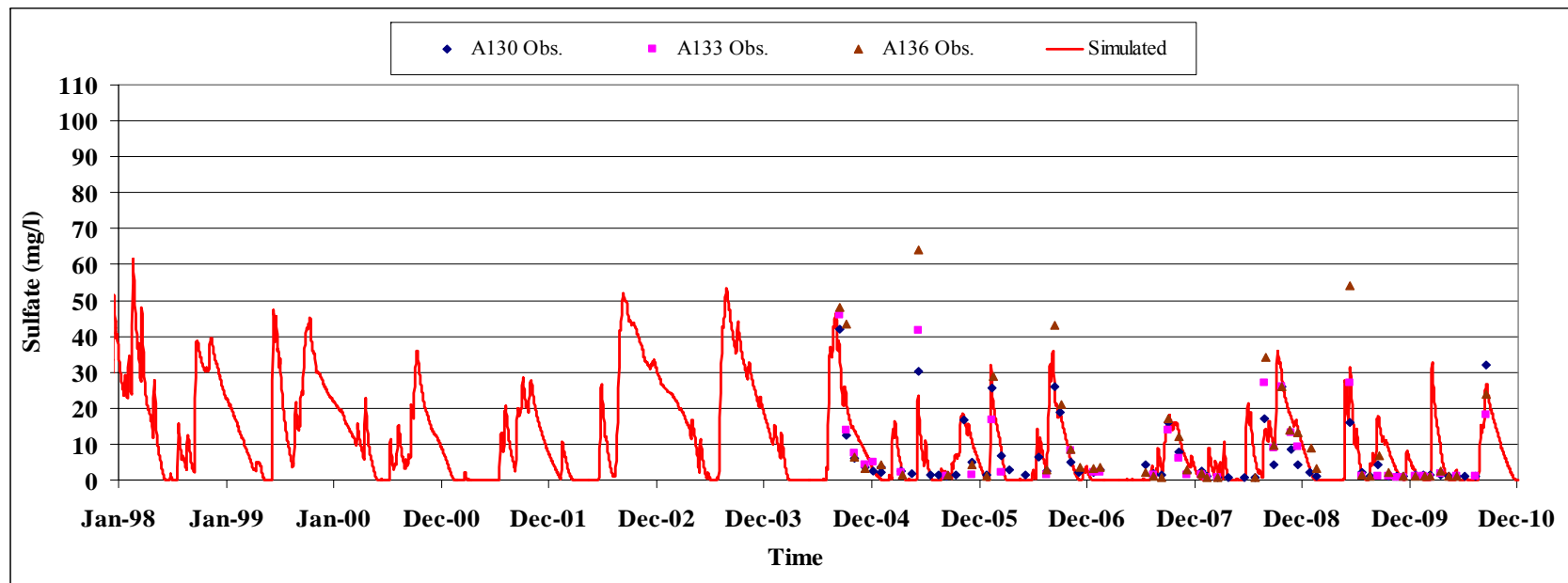


Figure 35 – Comparison of simulated sulfate concentration of M30 with observed data at stations within M30

Appendix E

Comparison of simulated total phosphorus with observed data within compartments

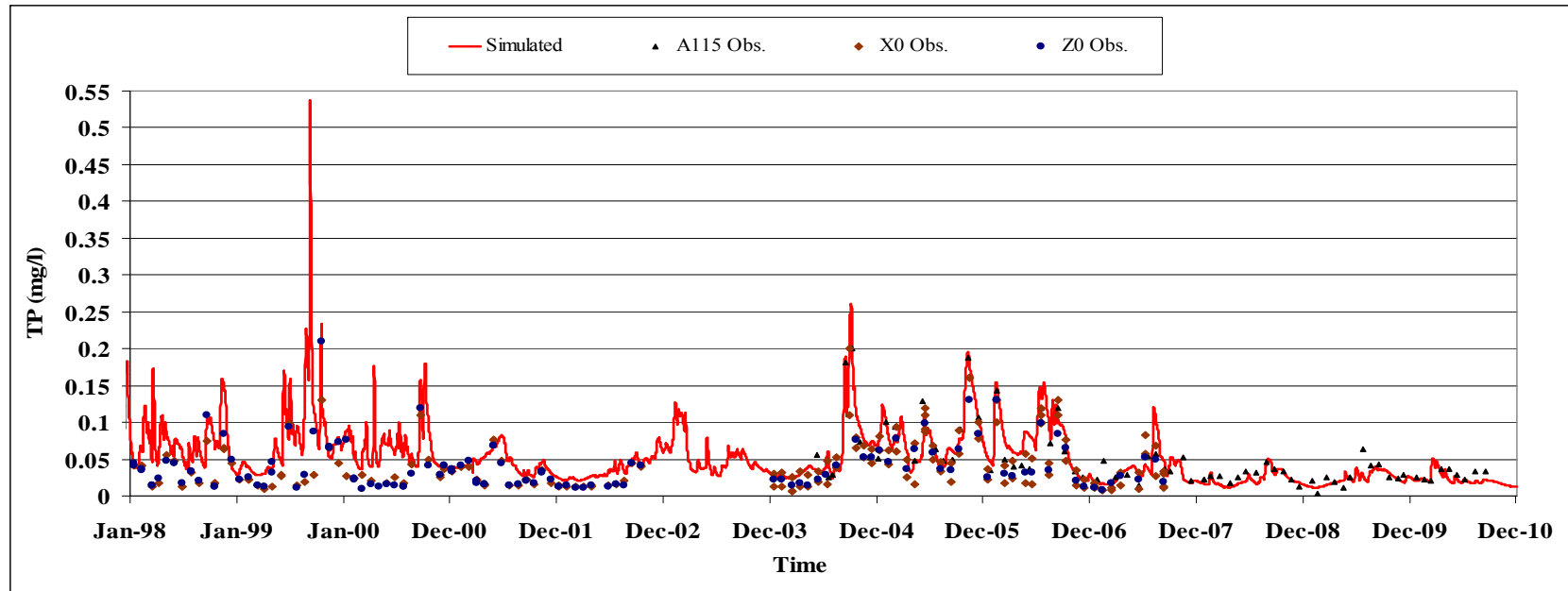


Figure 36 – Comparison of simulated total phosphorous concentration of C4 with observed data at stations within C4

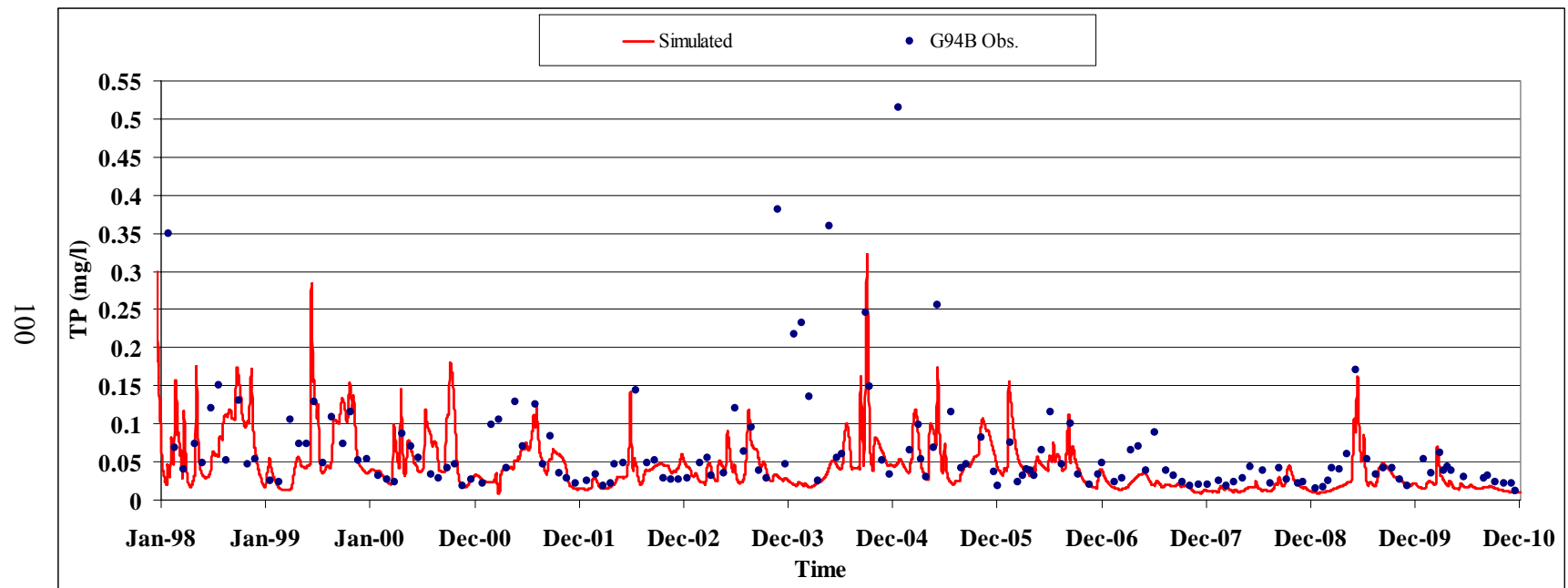


Figure 37 – Comparison of simulated total phosphorous concentration of C9 with observed data at stations within C9

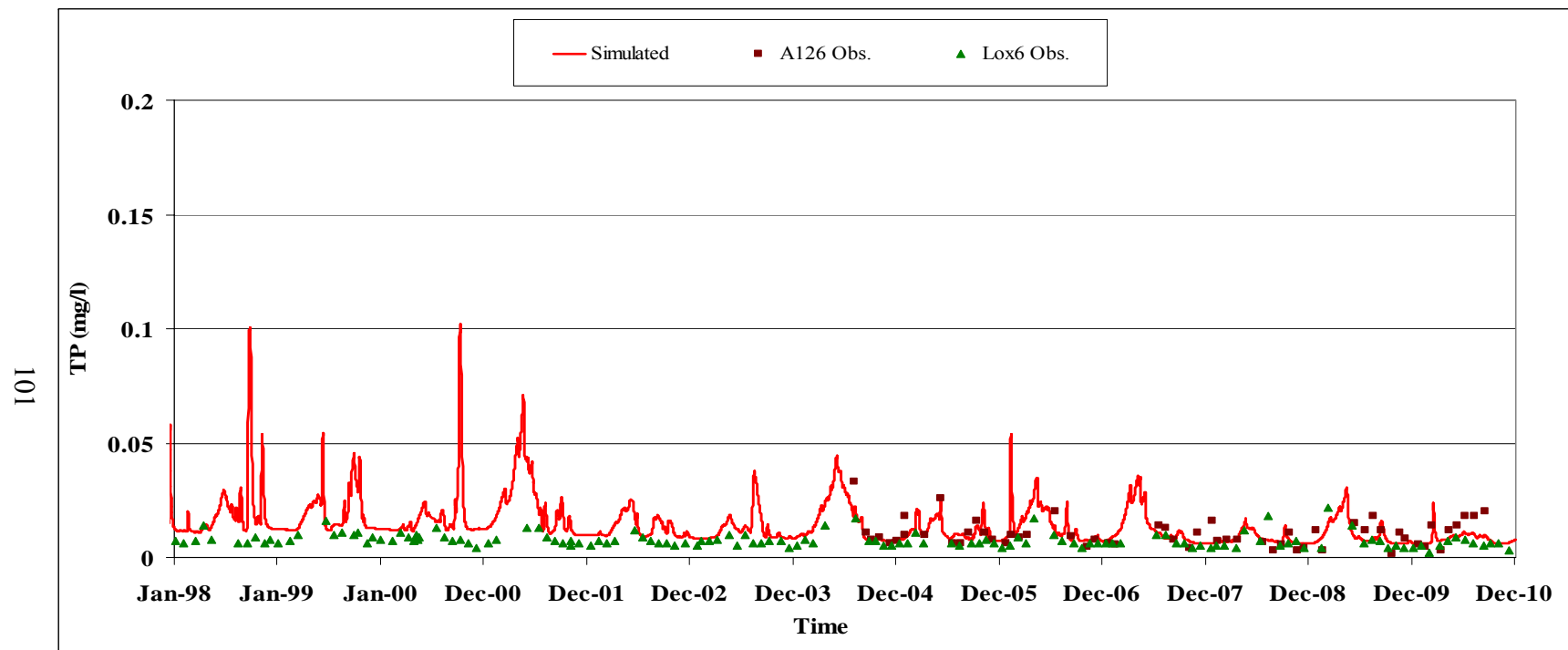


Figure 38 – Comparison of simulated total phosphorous concentration of M28 with observed data at stations within M28

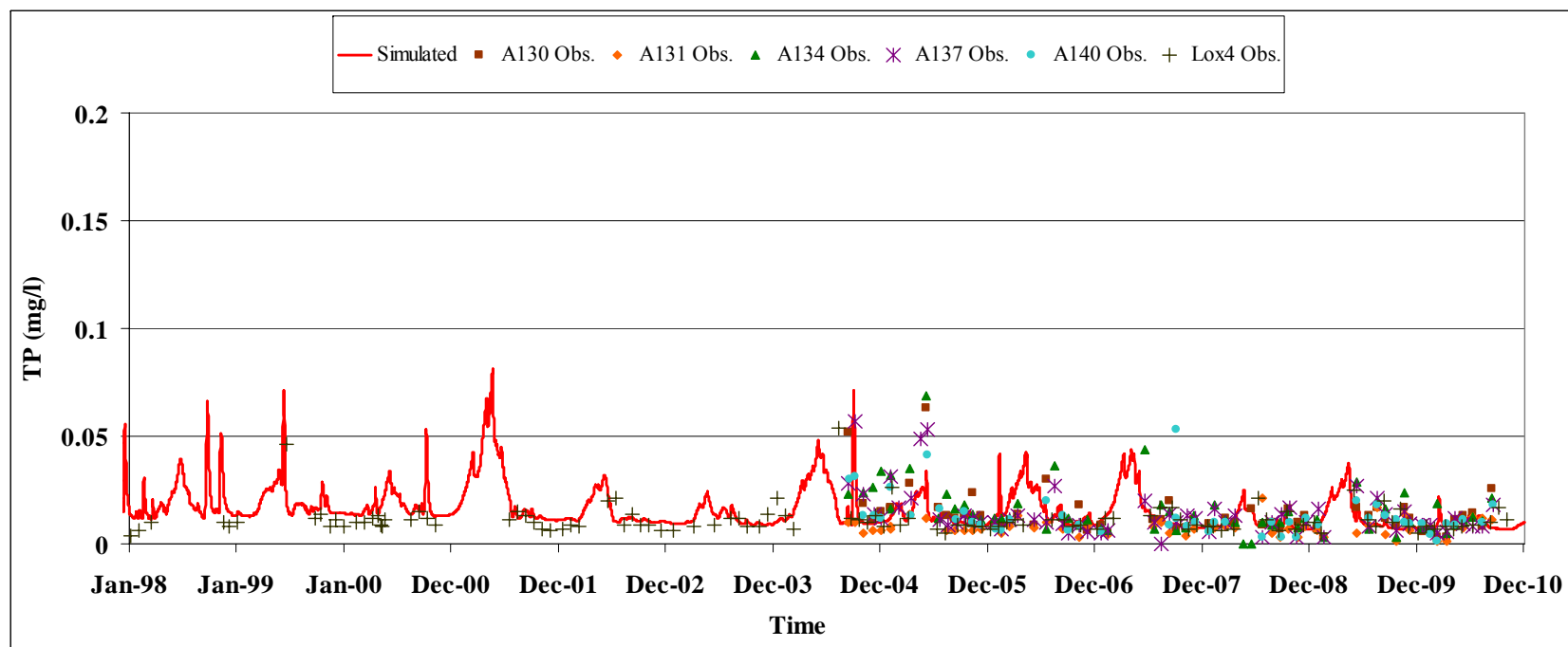


Figure 39 – Comparison of simulated total phosphorous concentration of M31 with observed data at stations within M31

Appendix F

Statistics presented in this appendix are for the selected two transects on the west and east side of the Refuge, for comparing the comparative analysis of 39-Compartment Model, (39-C) and Spatially Explicit Model, (MF) vs. observed data. ASC, ISC, and MAC are representing Aggregated Site Comparison, Individual Site Comparison, and Mesh Average Comparison sequentially.

Comparison Method	ASC	ASC	MAC	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC
Site ID				A115	X0	Z0	S10E	A115	X0	Z0	S10E
Model	39-C	MF	MF	39-C	39-C	39-C	39-C	MF	MF	MF	MF
Bias (mg/L)	-5.13	3.09	2.44	-2.70	-9.28	-7.82	5.45	6.89	-1.16	-0.22	8.13
Ave. Obs (mg/L)	107.89	107.89	107.89	100.12	113.61	112.23	116.78	100.12	113.61	112.23	116.78
Ave. Sim (mg/L)	102.76	110.98	110.33	97.42	104.34	104.41	122.23	107.01	112.45	112.01	124.91
RMSE (mg/L)	22.21	19.55	19.07	21.86	23.21	23.49	14.72	20.44	18.84	19.40	17.30
STD Obs. (mg/L)	37.92	37.92	37.92	39.58	37.42	36.67	28.64	39.58	37.42	36.67	28.64
STD Sim. (mg/L)	37.29	42.19	41.95	35.34	39.03	40.02	27.07	41.56	43.52	44.25	33.99
STD Error (mg/L)	21.67	19.36	18.96	21.83	21.49	22.41	14.24	19.37	19.00	19.62	15.89
Variance Reduction	67%	74%	75%	70%	67%	63%	75%	76%	74%	71%	69%
R (Correl Coef)	0.83	0.89	0.89	0.84	0.84	0.83	0.87	0.89	0.90	0.90	0.88
R^2	0.70	0.79	0.80	0.70	0.71	0.69	0.76	0.79	0.81	0.81	0.78
Nash-Sutcliffe Eff	0.66	0.73	0.75	0.69	0.61	0.58	0.71	0.73	0.74	0.71	0.60

Table 12 – Comparison of statistics of chloride concentration in C4 for 1/1/2004 to 12/31/2010

Comparison Method	ASC	ASC	MAC	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC
Site ID				A121	X1	Z1	A116	A121	X1	Z1	A116
Model	39-C	MF	MF	39-C	39-C	39-C	39-C	MF	MF	MF	MF
Bias (mg/L)	-32.62	12.76	7.93	-32.78	-30.56	-40.30	-26.14	17.05	16.79	2.35	19.19
Ave. Obs (mg/L)	101.18	101.18	101.18	100.49	105.89	110.06	88.11	100.49	105.89	110.06	88.11
Ave. Sim (mg/L)	68.56	113.94	109.11	67.71	75.33	69.75	61.97	117.54	122.68	112.41	107.31
RMSE (mg/L)	43.36	25.21	22.22	43.88	42.49	49.27	36.74	25.72	26.13	21.70	27.61
STD Obs. (mg/L)	40.19	40.19	40.19	40.11	41.30	37.66	40.21	40.11	41.30	37.66	40.21
STD Sim. (mg/L)	28.79	40.31	40.74	22.72	29.87	31.28	26.33	31.06	42.94	38.82	42.20
STD Error (mg/L)	28.70	21.84	20.86	30.75	30.07	28.74	26.20	20.29	20.40	21.88	20.15
Variance Reduction	49%	70%	73%	41%	47%	42%	58%	74%	76%	66%	75%
R (Correl Coef)	0.70	0.85	0.87	0.65	0.69	0.67	0.77	0.87	0.88	0.84	0.88
R^2	0.49	0.73	0.75	0.42	0.47	0.44	0.59	0.75	0.78	0.70	0.78
Nash-Sutcliffe Eff	-0.18	0.60	0.69	-0.33	-0.10	-0.76	0.14	0.54	0.58	0.66	0.51

Table 13 – Comparison of statistics of chloride concentration in M18 for 1/1/2004 to 12/31/2010

Comparison Method	ASC	ASC	MAC	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC
Site ID				A117	A122	X2	Z2	A117	A122	X2	Z2
Model	39-C	MF	MF	39-C	39-C	39-C	39-C	MF	MF	MF	MF
Bias (mg/L)	-4.44	8.57	-8.75	-3.29	-8.21	-0.70	-13.91	10.99	3.80	9.13	-1.80
Ave. Obs (mg/L)	61.72	61.73	61.72	54.25	57.49	61.88	73.00	54.25	57.49	61.88	73.00
Ave. Sim (mg/L)	57.28	70.30	52.96	50.97	49.27	61.18	59.09	65.24	61.29	71.01	71.20
RMSE (mg/L)	25.11	30.98	25.19	21.95	25.16	28.48	22.14	28.62	33.11	32.17	32.11
STD Obs. (mg/L)	36.67	36.78	36.67	34.02	32.78	39.19	33.80	34.02	32.78	39.19	33.80
STD Sim. (mg/L)	29.04	41.53	29.66	21.37	22.32	31.46	33.52	40.23	43.36	44.06	42.41
STD Error (mg/L)	24.79	29.86	23.69	21.90	23.99	28.87	17.47	26.66	33.19	31.28	32.52
Variance Reduction	54%	34%	58%	59%	46%	46%	73%	39%	-2%	36%	7%
R (Correl Coef)	0.74	0.72	0.76	0.78	0.68	0.69	0.87	0.75	0.65	0.72	0.66
R^2	0.55	0.51	0.58	0.61	0.46	0.47	0.75	0.57	0.42	0.52	0.43
Nash-Sutcliffe Eff	0.53	0.29	0.53	0.58	0.40	0.46	0.56	0.28	-0.04	0.31	0.07

Table 14 – Comparison of statistics of chloride concentration in M19 for 1/1/2004 to 12/31/2010

Comparison Method	ASC	ASC	MAC	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC
Site ID				A111	112	A113	A114	A118	A119	A120	A128
Model	39-C	MF	MF	39-C	39-C	39-C	39-C	39-C	39-C	39-C	39-C
Bias (mg/L)	2.23	-0.75	-6.59	4.26	-2.56	3.60	3.22	-2.52	6.59	-0.14	2.30
Ave. Obs (mg/L)	24.60	24.02	24.02	18.18	26.33	18.99	18.11	26.99	18.18	24.00	19.33
Ave. Sim (mg/L)	26.83	23.25	17.40	22.44	23.77	22.59	21.33	24.47	24.76	23.86	21.63
RMSE (mg/L)	16.27	15.27	13.70	11.12	17.47	12.09	10.98	15.57	12.54	14.34	11.71
STD Obs. (mg/L)	12.99	12.52	12.52	8.34	16.45	7.90	5.42	16.76	5.93	10.94	6.16
STD Sim. (mg/L)	19.17	20.51	12.95	12.00	14.08	13.28	11.37	13.64	14.03	13.54	11.13
STD Error (mg/L)	16.12	15.26	12.02	10.37	17.44	11.65	10.60	15.49	10.76	14.44	11.59
Variance Reduction	-54%	-49%	8%	-54%	-12%	-117%	-283%	15%	-229%	-74%	-255%
R (Correl Coef)	0.55	0.67	0.56	0.53	0.36	0.49	0.38	0.50	0.70	0.32	0.20
R^2	0.31	0.45	0.31	0.28	0.13	0.24	0.14	0.25	0.49	0.10	0.04
Nash-Sutcliffe Eff	-0.57	-0.48	-0.19	-0.81	-0.15	-1.39	-3.19	0.12	-3.55	-0.74	-2.69

Table 15 – Comparison of statistics of chloride concentration in M36 for 1/1/2004 to 12/31/2010

Comparison Method	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC
Site ID	lox 9	lox 10	lox 12	X3	X4	Y4	Z3	Z4	A111	112	A113
Model	39-C	39-C	39-C	39-C	39-C	39-C	39-C	39-C	MF	MF	MF
Bias (mg/L)	2.00	5.30	1.69	0.79	4.92	5.06	-1.94	4.24	-0.46	0.86	-2.73
Ave. Obs (mg/L)	23.28	21.83	26.83	34.82	29.06	29.14	36.03	29.96	18.18	26.33	18.28
Ave. Sim (mg/L)	25.28	27.13	28.52	35.61	33.98	34.20	34.09	34.20	17.72	27.19	15.55
RMSE (mg/L)	18.38	15.13	18.09	17.17	21.67	21.08	17.78	22.79	13.53	20.16	13.40
STD Obs. (mg/L)	7.53	10.96	11.10	20.17	15.08	13.89	16.83	10.23	8.34	16.45	7.10
STD Sim. (mg/L)	19.21	19.58	20.67	26.75	26.52	26.68	26.22	26.68	16.55	23.77	14.71
STD Error (mg/L)	18.43	14.29	18.13	17.37	21.35	20.71	17.87	22.67	13.66	20.32	13.24
Variance Reduction	-498%	-70%	-167%	26%	-101%	-122%	-13%	-391%	-168%	-53%	-248%
R (Correl Coef)	0.30	0.70	0.48	0.76	0.59	0.64	0.74	0.56	0.57	0.54	0.44
R^2	0.09	0.49	0.23	0.58	0.35	0.41	0.54	0.31	0.32	0.29	0.19
Nash-Sutcliffe Eff	-5.05	-0.94	-1.69	0.26	-1.11	-1.36	-0.14	-4.09	-1.68	-0.53	-2.63

Table 15 continued – Comparison of statistics of chloride concentration in M36 for 1/1/2004 to 12/31/2010

Comparison Method	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC
Site ID	A114	A118	A119	A120	A128	lox 9	lox 10	lox 12	X3	X4	Y4	Z3	Z4
Model	MF	MF	MF	MF	MF	MF	MF	MF	MF	MF	MF	MF	MF
Bias (mg/L)	-5.09	3.70	2.00	-8.35	-6.87	-10.47	2.47	-1.31	7.28	4.19	6.48	4.36	1.50
Ave. Obs (mg/L)	18.11	26.83	17.63	24.00	19.33	23.28	21.68	26.83	32.33	29.06	25.44	34.99	28.91
Ave. Sim (mg/L)	13.02	30.53	19.63	15.66	12.45	12.81	24.15	25.52	39.61	33.26	31.92	39.35	30.41
RMSE (mg/L)	11.48	17.09	11.84	13.01	12.68	15.56	16.03	13.31	21.08	19.86	16.82	14.58	13.75
STD Obs. (mg/L)	5.42	16.86	5.49	10.94	6.16	7.53	10.99	11.10	19.57	15.08	10.51	16.77	9.79
STD Sim. (mg/L)	11.08	22.93	14.70	12.36	10.38	12.12	21.48	18.85	26.61	27.99	20.93	23.68	19.69
STD Error (mg/L)	10.39	16.82	11.77	10.05	10.77	11.61	15.96	13.33	20.08	19.64	15.74	14.08	13.84
Variance Reduction	-268%	0%	-359%	16%	-206%	-137%	-111%	-44%	-5%	-70%	-124%	30%	-100%
R (Correl Coef)	0.37	0.68	0.67	0.63	0.23	0.38	0.69	0.72	0.66	0.74	0.68	0.81	0.76
R^2	0.14	0.46	0.44	0.40	0.05	0.14	0.48	0.52	0.44	0.55	0.47	0.66	0.57
Nash-Sutcliffe Eff	-3.58	-0.04	-3.73	-0.43	-3.33	-3.34	-1.16	-0.46	-0.19	-0.78	-1.63	0.23	-1.02

Table 15 continued – Comparison of statistics of chloride concentration in M36 for 1/1/2004 to 12/31/2010

Comparison Method	ASC	ASC	MAC	ISC	ISC	ISC	ISC	ISC	ISC
Site ID				A129	A132	A135	A129	A132	A135
Model	39-C	MF	MF	39-C	39-C	39-C	MF	MF	MF
Bias (mg/L)	-11.17	-3.83	-3.29	-5.47	-11.07	-16.98	-3.96	-2.20	-5.32
Ave. Obs (mg/L)	93.29	93.29	93.29	87.34	93.13	99.39	87.34	93.13	99.39
Ave. Sim (mg/L)	82.12	89.46	90.00	81.87	82.06	82.42	83.38	90.93	94.07
RMSE (mg/L)	27.04	26.50	26.04	25.48	27.05	28.51	26.38	25.50	27.59
STD Obs. (mg/L)	31.89	31.89	31.89	30.96	31.77	32.20	30.96	31.77	32.20
STD Sim. (mg/L)	26.93	37.56	36.71	27.36	27.04	26.77	38.74	37.33	36.28
STD Error (mg/L)	24.68	26.28	25.89	25.05	24.84	23.06	26.25	25.58	27.25
Variance Reduction	40%	32%	34%	35%	39%	49%	28%	35%	28%
R (Correl Coef)	0.66	0.73	0.72	0.64	0.65	0.71	0.74	0.74	0.69
R^2	0.44	0.53	0.52	0.41	0.43	0.50	0.54	0.54	0.48
Nash-Sutcliffe Eff	0.28	0.31	0.33	0.31	0.27	0.21	0.26	0.35	0.26

Table 16 – Comparison of statistics of chloride concentration in C10 for 1/1/2004 to 12/31/2010

Comparison Method	ASC	ASC	MAC	ISC	ISC	ISC	ISC	ISC	ISC
Site ID				A130	A133	A136	A130	A133	A136
Model	39-C	MF	MF	39-C	39-C	39-C	MF	MF	MF
Bias (mg/L)	-8.36	-15.11	0.97	-7.03	-5.37	-12.52	-15.50	-12.07	-16.59
Ave. Obs (mg/L)	55.99	55.43	55.99	53.43	55.06	60.04	52.01	55.06	60.04
Ave. Sim (mg/L)	47.63	39.95	56.96	46.40	49.69	47.52	36.51	41.65	42.25
RMSE (mg/L)	23.16	24.53	25.81	23.92	21.37	23.59	23.27	24.30	25.99
STD Obs. (mg/L)	30.42	29.72	30.42	31.57	29.43	29.92	29.75	29.43	29.92
STD Sim. (mg/L)	19.97	27.04	32.17	21.22	20.61	17.93	26.58	26.54	28.16
STD Error (mg/L)	21.67	19.38	25.88	23.05	20.94	20.19	17.50	21.36	20.20
Variance Reduction	49%	57%	28%	47%	49%	54%	65%	47%	54%
R (Correl Coef)	0.70	0.77	0.66	0.68	0.70	0.75	0.81	0.71	0.76
R^2	0.49	0.59	0.43	0.47	0.49	0.57	0.66	0.51	0.58
Nash-Sutcliffe Eff	0.42	0.33	0.28	0.42	0.46	0.37	0.38	0.34	0.27

Table 17 – Comparison of statistics of chloride concentration in M30 for 1/1/2004 to 12/31/2010

Comparison Method	ASC	ASC	MAC	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC
Site ID				A130	A131	A134	A137	A140	Lox4	A130	A131
Model	39-C	MF	MF	39-C	39-C	39-C	39-C	39-C	39-C	MF	MF
Bias (mg/L)	-5.05	-10.18	-9.63	-14.10	6.00	-10.00	-7.32	3.15	-6.23	-15.50	-7.26
Ave. Obs (mg/L)	45.22	44.82	45.22	53.43	34.03	49.50	46.53	38.13	48.06	52.01	34.03
Ave. Sim (mg/L)	40.17	34.64	35.59	39.33	40.03	39.49	39.21	41.28	41.83	36.51	26.77
RMSE (mg/L)	23.45	22.32	22.52	27.63	20.48	25.20	23.42	18.95	23.18	23.27	15.31
STD Obs. (mg/L)	26.05	25.72	26.05	31.57	18.97	28.34	26.89	20.59	22.57	29.75	18.97
STD Sim. (mg/L)	18.03	24.66	22.35	18.02	17.86	18.24	18.26	17.32	18.83	26.58	19.11
STD Error (mg/L)	22.94	19.89	20.38	23.95	19.74	23.32	22.43	18.87	22.50	17.50	13.59
Variance Reduction	23%	40%	39%	42%	-8%	32%	30%	16%	1%	65%	49%
R (Correl Coef)	0.51	0.69	0.66	0.66	0.43	0.57	0.56	0.52	0.42	0.81	0.75
R^2	0.26	0.47	0.43	0.43	0.18	0.33	0.32	0.27	0.18	0.66	0.56
Nash-Sutcliffe Eff	0.19	0.24	0.25	0.22	-0.18	0.20	0.23	0.14	-0.07	0.38	0.34

Table 18 – Comparison of statistics of chloride concentration in M31 for 1/1/2004 to 12/31/2010

Comparison Method	ISC	ISC	ISC	ISC
Site ID	A134	A137	A140	Lox4
Model	MF	MF	MF	MF
Bias (mg/L)	-11.50	-10.78	-8.08	-6.54
Ave. Obs (mg/L)	48.91	45.75	37.67	48.06
Ave. Sim (mg/L)	36.61	34.97	29.60	41.51
RMSE (mg/L)	25.87	23.09	20.94	23.97
STD Obs. (mg/L)	28.21	26.90	21.37	22.57
STD Sim. (mg/L)	24.79	23.86	18.92	29.00
STD Error (mg/L)	23.37	20.59	19.55	23.24
Variance Reduction	31%	41%	16%	-6%
R (Correl Coef)	0.65	0.68	0.53	0.62
R^2	0.43	0.46	0.29	0.38
Nash-Sutcliffe Eff	0.17	0.25	0.02	-0.15

Table 18 continued – Comparison of statistics of chloride concentration in M31 for 1/1/2004 to 12/31/2010

Comparison Method	ASC	ASC	MAC	ISC	ISC	ISC	ISC	ISC	ISC	ISC	ISC
Site ID				Lox3	Lox5	A138	A139	Lox3	Lox5	A138	A139
Model	39-C	MF	MF	39-C	39-C	39-C	39-C	MF	MF	MF	MF
Bias (mg/L)	-4.82	-5.17	-5.06	-1.60	-2.12	-12.54	-0.87	-7.50	-9.67	-3.06	-2.93
Ave. Obs (mg/L)	23.17	23.69	23.17	19.58	20.57	31.41	18.78	19.58	19.01	31.41	18.99
Ave. Sim (mg/L)	18.35	18.51	18.11	17.98	18.45	18.86	17.91	12.08	9.34	28.34	16.07
RMSE (mg/L)	14.37	12.37	13.44	10.46	10.03	21.01	10.53	11.32	12.27	14.26	10.08
STD Obs. (mg/L)	12.26	13.11	12.26	5.19	6.13	17.81	7.37	5.19	5.16	17.81	7.42
STD Sim. (mg/L)	11.29	15.83	11.78	10.28	10.39	12.81	11.40	7.63	5.89	19.91	11.13
STD Error (mg/L)	13.58	11.27	12.48	10.47	9.91	17.00	10.61	8.59	7.71	14.05	9.79
Variance Reduction	-23%	26%	-4%	-307%	-162%	9%	-107%	-174%	-124%	38%	-74%
R (Correl Coef)	0.34	0.71	0.46	0.22	0.37	0.42	0.43	0.14	0.03	0.73	0.50
R^2	0.11	0.51	0.21	0.05	0.14	0.18	0.18	0.02	0.00	0.53	0.25
Nash-Sutcliffe Eff	-0.38	0.10	-0.21	-3.16	-1.74	-0.42	-1.09	-3.88	-4.91	0.35	-0.90

Table 19 – Comparison of statistics of chloride concentration in M35 for 1/1/2004 to 12/31/2010

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Bazgirkhoob, Hamid. Bachelor of Science, Islamic Azad University–Shiraz Branch, July 2003; Master of Science, University of Louisiana at Lafayette, Summer 2012
Major: Engineering, Civil Engineering option
Title of Thesis: Stage and Water Quality Compartmental Model of an Everglades Wetland
Thesis Directors: Dr. Ehab Meselhe and Dr. Chunfang Chen
Pages in Thesis: 132; Words in Abstract: 336

Abstract

Cluster analysis was applied to objectively determine the number of compartments and to spatially delineate compartments with similar features in the Arthur R. Marshall Loxahatchee National Wildlife Refuge which led to delineate the 9-Compartment Model structure based on the analysis of concentrations of chloride, total phosphorus, sulfate, and calcium. The 39-Compartment Model was built by analyzing the water quality gradient from the calibration and validation of the 9-Compartment Model, and professional judgment by analyzing information such as the vegetation/elevation map of the Refuge.

The 39-Compartment Model results represent spatially aggregated canal and marsh values for all state variables (e.g., volume, stage, and water quality parameters). The 39-Compartment Model predicts water stage very well for canal and marsh. The model also predicts the concentration of three constituents (Cl, SO₄, and TP) reasonably well. It is evinced that in the Refuge, the inflow structures in the north have strong impact to the flows in the canal and the northern marsh. Automated calibration of the seepage coefficients for the marsh and the canal revealed that the seepage loss in canals for the 39-Compartment Model is larger than that for the 9-Compartment Model.

The 39-Compartment Model and the Spatially Explicit Model (Mike Flood) were quantitatively evaluated vs. observed data. Although, the 39-Compartment Model can be

used to detect water quality variations along western and eastern gradients as well as north-to-south gradient, due to its spatially aggregated nature, the model is not desired be used to analyze site specific events. But, the Spatially Explicit Model (Mike Flood) can provide more accurate prediction to the observed data for the Refuge. The Spatially Explicit Model results provide detailed spatial and temporal information of hydrodynamic and water quality state variables. This model can be used to analyze site specific events. Depending on the time scale of input data, Mike Flood can be used for analyzing short term (transient) to long term (daily, monthly or annual) events. In view of its computational cost, it is feasible to run decadal simulation within reasonable amount of time.

Biographical Sketch

Hamid Bazgirkhoob was born on August 8, 1980 in Shiraz, Iran to Abdolhossein Bazgirkhoob and Zohreh Tavallaei. He attended Islamic Azad University in Shiraz, Iran where he earned a Bachelor of Science in Irrigation Engineering. After graduation, he was employed in water resources consulting firms, primarily in channel/canal/pipe distribution networks. He started his master's program under supervision of Dr. Ehab Meselhe at the University of Louisiana at Lafayette in August of 2010, and will complete degree requirements for a Master of Science in Engineering, Civil Engineering option in the summer of 2012.