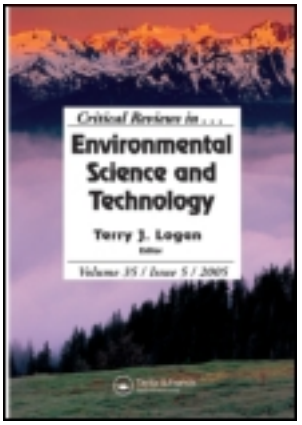


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# Mechanistic Biogeochemical Model Applications for Everglades Restoration: A Review of Case Studies and Suggestions for Future Modeling Needs

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# Mechanistic Biogeochemical Model Applications for Everglades Restoration: A Review of Case Studies and Suggestions for Future Modeling Needs

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*Mechanistic biogeochemical model applications for freshwater wetland ecosystems are reviewed with an emphasis on applications in the Florida Everglades. Two significant human impacts on the Everglades have been hydrologic alteration and phosphorus (P) enrichment. Thus, it is important for research conducted in support of Everglades restoration to integrate understanding of the coupled effects of hydrologic and biogeochemical processes. Models are tools that can facilitate such integration, but an important challenge in model development is determining the appropriate level of model complexity. Previous wetland biogeochemical and flow modeling efforts are categorized across the spectrum of complexity from empirical and spatially aggregated to mechanistic and spatially distributed. The focus of this review is on mercury and P, as these two elements represent major environmental concerns in this ecosystem. Two case studies of coupled hydrologic and biogeochemical modeling for P transport are described in further detail to illustrate the implications of different levels of model complexity. The case study simulation results on time series TP data revealed that the mechanistic biogeochemical model with more complexity did not guarantee significantly better simulation accuracy compared to the simpler one. It is concluded that the level of model complexity should be represented appropriately based on the modeling objectives, hypotheses to be tested, and data availability. Finally, better integration between data collection and model development*

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*is encouraged as cross-fertilization between these processes may stimulate improved system understanding.*

**KEYWORDS:** biogeochemical model, Everglades, mechanistic model, phosphorus cycling, restoration, wetland

## 1 INTRODUCTION

Mechanistic biogeochemical models have been extensively applied to diverse aquatic ecosystems including rivers, lakes, wetlands, and estuaries (Chen and Sheng, 2005; Jørgensen and Bendoricchio, 2001; Robson et al., 2008). Such modeling is a core research tool to support understanding ecosystem structures and functions, and support management decision making through hypothesis testing and prediction (Arhonditsis et al., 2006, 2008; Mitsch and Reeder, 1991; Sklar et al., 2001; Wang and Mitsch, 2000). Historically, the Florida Everglades was a huge oligotrophic freshwater wetland ecosystem that extended from the upper basin of the Kissimmee River to the Florida Bay. However, more than a century of human intervention has degraded this unique wetland area. Hydrologic alteration and phosphorus (P) rich surface runoff have been designated as the two most fundamental causes of major environmental issues in the Everglades over the last several decades (Newman and Lynch, 2001). Thus, it is important for research conducted in support of Everglades restoration to integrate understanding of the coupled effects of hydrologic and biogeochemical processes. Models are tools that can facilitate such integration for understanding process behavior, designing engineered systems (such as the large treatment wetlands known as stormwater treatment areas [STAs]), and evaluating scenarios that cannot be easily tested physically.

The spectrum of complexity of hydrologic and biogeochemical representations in wetland modeling is categorized conceptually in Figure 1. For biogeochemical modeling, the simplest approaches use empirical or process-lumped equations. More complex models adapt physical process-based mechanistic or ecosystem-level compartment modeling approaches. For flow modeling, the simple and complex approaches can be generally classified in terms of time (steady state vs. transient) or space (spatially aggregated vs. distributed). Here, the four different combinations of these characteristics describing the integration between hydrologic and biogeochemical models (Figure 1) are used to categorize the case studies reviewed. Although this classification is a simplification of the possible spectrum of coupled hydrologic-biogeochemical wetland modeling, it facilitates comparison of modeling approach strengths and weaknesses, and helps understand individual case studies within the broader context of possible modeling approaches. Thus, this classification was used here to review the present status

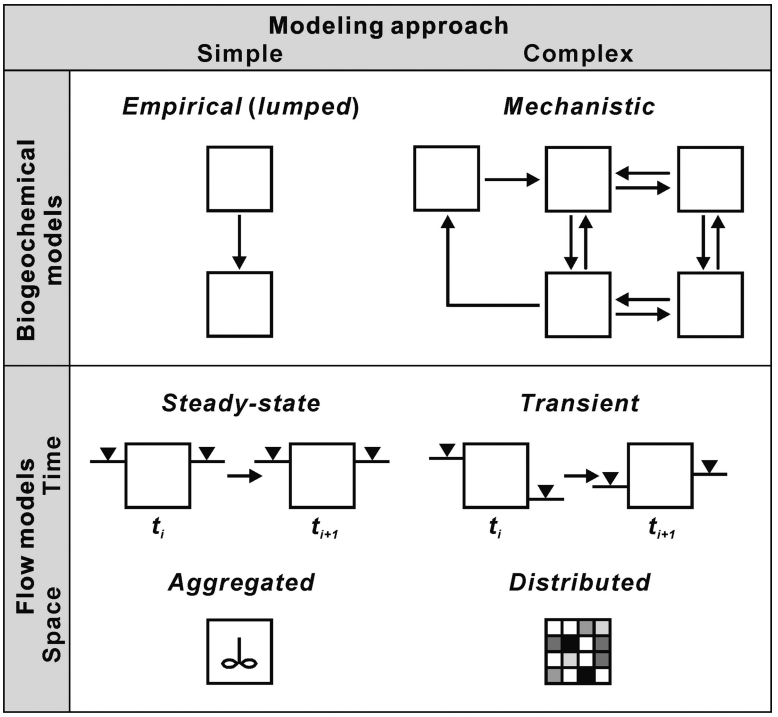


**FIGURE 1.** Conceptual diagram of approaches for incorporating biogeochemical and flow complexity in wetland modeling.

of mechanistic biogeochemical model applications for freshwater wetland ecosystems, with an emphasis on mercury (Hg) and P in the Florida Everglades. These two elements represent major environmental concerns in this ecosystem, and to our knowledge mechanical biogeochemical modeling efforts on other constituents such as C, N, heavy metals, and organic compounds have been rarely reported (Browder and Volk, 1978; Kadlec and Wallace, 2009; Martin and Reddy, 1997).

Some historical empirical (relatively simple and parameter-lumped) biogeochemical models have been very useful as management modeling tools and predictive tools for treatment wetlands and of long-term P retention. However, more mechanistic (relatively complex and process-based) biogeochemical modeling approaches may be necessary to systematically understand the internal processes of a wetland ecosystem and predict the biogeochemical impacts as a result of changes in environmental factors such as hydrology and climate. This modeling approach is also essential to achieve the goals of the Everglades restoration.

Since the promulgation of the 1994 Everglades Forever Act, rigorous ecosystem restoration efforts have been carried out in Florida through various regulatory, research, and construction activities. One of the primary efforts

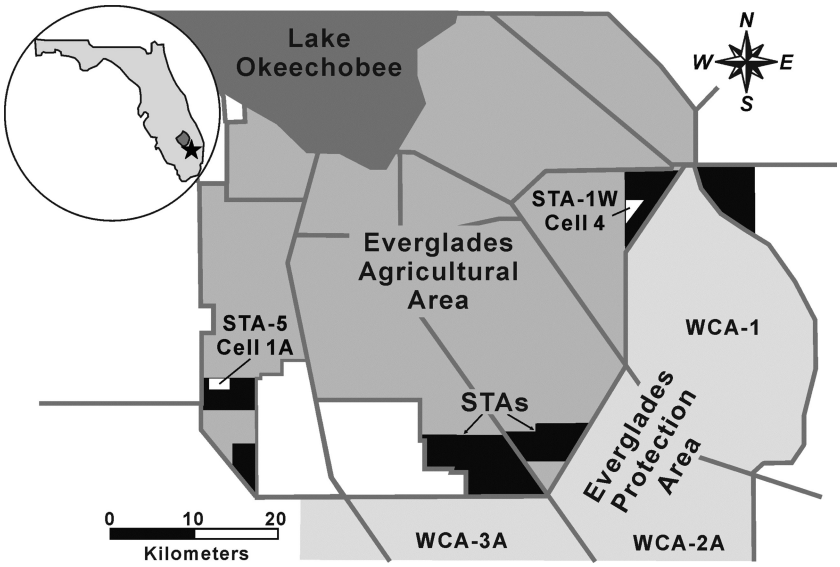


**FIGURE 2.** Regional map showing the strategic locations of STAs and two treatment cells selected for case studies: STA-1W Cell 4 and STA-5 Cell 1A.



was construction of the STAs strategically located between the Everglades Agricultural Area and Everglades Protection Area (Water Conservation Areas [WCAs]; Figure 2). The STAs comprise the largest treatment wetland system in the world (total effective treatment area of approximately 182 $km^2$) and have played a critical role in reducing P levels in surface water entering the EPA. Through two case studies applied in the Everglades, we examine the level of complexity and model performance of two mechanistic P models that were applied to the STAs.

Our focus in this paper was not to fully describe the model development processes, algorithms used, and the major conclusions elicited from the modeling efforts, but to review mechanistic biogeochemical modeling approaches in terms of the flow and P-dynamics complexity levels described in Figure 1. The emphasis was on examples in the Florida Everglades, but also included discussion of applications in other areas that have potential to be applied for this wetland ecosystem. In addition, we contrasted two P models in terms of level of complexity and the associated model prediction performances on the time series outlet TP concentration profiles. Therefore, the specific objectives of this communication were to (a) estimate an optimized level of mechanistic biogeochemical model complexity based on present data availability and (b) identify major data gaps and modeling needs essential for development of more advanced mechanistic biogeochemical models to support Everglades restoration.

## 2 MECHANISTIC MODELING APPROACHES

A fundamental challenge for wetland scientists is determining the appropriate level of complexity for biogeochemical models to effectively simulate the fate and behavior of target elements in wetlands. For example, many researchers have developed and applied wetland P models of widely varying complexity in flow as well as in the cycling (Table 1) to address varying objectives. Empirical biogeochemical modeling approaches are relatively easy to develop and apply, but only provide relationships among observational data. Empirical models are useful in describing an overall trend in a system but do not have mechanistic relevance. The advantages of empirical modeling approaches conversely become the disadvantages of mechanistic modeling approaches. Fernandez et al. (2006) summarized the shortcomings of mechanistic approaches: (a) they usually require extensive model input data and physical parameters—in many cases, some of the model input data or parameters are not available, which makes it difficult to develop



**TABLE 1.** Wetland P model classification in terms of level of complexity on flow and P dynamics

| | P dynamics | |
|---|---|---|
| Flow | More empirical | More mechanistic |
| Fully assumed | *Empirical mass balance approach*<br>• Kadlec and Newman (1992)<br>• Kadlec and Wallace (2009)<br>*First-order kinetic or Vollenweider type approach*<br>• Kadlec (1994)<br>• Mitsch et al. (1995)<br>• Reed et al. (1995)<br>• Walker (1995)<br>• Kadlec and Wallace (2009)<br>• Wong and Geiger (1997)<br>• Kadlec (2000)<br>• Carleton et al. (2001)<br>• Black and Wise (2003)<br>• Wang and Jawitz (2006)<br>• Chavan and Dennett (2008) | *Ditch*<br>• Janse (1998)<br>*River marginal wetlands*<br>• van der Peijl and Verhoeven (1999)<br>*Everglades*<br>• Walker and Kadlec (1996; EPGM)<br>• Noe and Childers (2007; P budget) |
| Fully considered | *Watershed model-based approach*<br>• Huber and Dickinson (1988; SWMM)<br>• Arnold et al. (1994; SWAT)<br>• Refsgaard and Storm (1995; MIKE SHE)<br>• Bicknell et al. (1997; HSPF)<br>• SWET, Inc. (2006; WAM)<br>• Bingner and Theurer (2009; AnnAGNPS)<br>*Hydrodynamic model-based approach*<br>• Tsanis et al. (1998)<br>• Raghunathan et al. (2001)<br>• Kazezyilmaz-Alhan et al. (2007) | *Lake wetland*<br>• Kadlec and Hammer (1988)<br>• Mitsch and Reeder (1991)<br>*River marginal wetlands*<br>• Wang and Mitsch (2000)<br>*Everglades*<br>• HydroQual (1997; WWQM)<br>• Fitz and Sklar (1999; ELM)<br>• Chen and Sheng (2005; Lake Okeechobee)<br>• Walker and Kadlec (2005; DMSTA2)<br>• Min (2007; MIKE 21)<br>• Jawitz et al. (2008; RSM-WQ) |

the model, this also makes it difficult to calibrate and validate the model; (b) the underlying uncertainties in the parameterization lead to uncertainties in model prediction; and (c) time and effort required to run these models are considerable.

In contrast, mechanistic biogeochemical models are usually complex because these models are designed to produce quantitative outputs based on the understanding of underlying functional mechanisms of the processes (Robson et al., 2008). Construction of mechanistic models begins with conceptualization of a system, which involves representing the key system components and their linkages. The model structure is generally formulated in terms of stores and flows among the stores to describe the fate and behavior of elements of interest within an ecosystem. For example, in wetlands, P stocks are in the water column, biomass, and soil, and the flows are the cycling and the transformation of P in various forms between these stocks. Thus, mechanistic models explicitly represent the functionality of internal dynamics of a system and seek to describe the relationship between the phenomenon and underlying principle of cause. In addition, these models allow simulating the physical and biogeochemical behavior of target elements quantitatively within a system and the physical meanings of model parameters are usually clear.

In ecosystem modeling, mechanistic models have formed the scientific basis in the decision making process by providing linkage between management questions and the response of the ecosystem (Arhonditsis et al., 2006; Fitz and Sklar, 1999; Fitz and Trimble, 2006; Walker and Kadlec, 2005). A key advantage of mechanistic models is that the variables in an ecosystem are mechanistically connected with the physical process-based linkages. Thus, such models have the ability to predict alternate management scenarios, which is critical to make management decisions. Spatially distributed models have added advantages because these models represent ecological processes throughout the simulated domain, enabling assessment of spatial variability of internal changes within the system as well as the effects of system inputs on outputs. In South Florida, several models have been used to simulate management strategies to adaptively guide the restoration and protection of the Everglades. For example, a Dynamic Model for Stormwater Treatment Areas (DMSTA) has been used for evaluating scenarios related to STAs and reservoirs under the Comprehensive Everglades Restoration Plan (CERP; Walker and Kadlec, 2005). Also, the Everglades Landscape Model (ELM) has been used to quantify potential ecosystem responses to altered hydrologic and nutrient drivers (Fitz and Trimble, 2006).

Mechanistic models are based on the underlying physics and chemistry governing the process and seek to describe phenomena with transferable equations that can be used predictively. This approach is contrasted with empirical methods that are based on observed relationships between variables that may not be transferable in space or time. The first step in developing a

mechanistic model is to construct a conceptual model that defines the key interactions between process variables based on fundamental knowledge. Then, each interaction is defined mathematically (e.g., first-order kinetic and Monod equation). Parameters for these relationships must be obtained from experimental data or field measurement. Finally the model should be validated against process data. Although these four steps in the model development are generally similar whether the model is empirical or mechanistic, the differences appear in resilience to perturbations. For example, if an empirical model parameter (e.g., settling coefficient) is a function of load or vegetation community, then the parameter must be changed when these input conditions change (Kadlec, 2000).

The level of complexity in mechanistic biogeochemical models is based on the goal or utility of the modeling effort. This is usually dependent on how much data are available for model fitting, but it is definitely based on what predictions are desired (e.g., What if the external load is directly reduced?) or what hypotheses can be tested (What about the effects of other key controlling parameters regulating the target component?). In reality, it is not always possible to completely differentiate mechanistic and empirical modeling approaches because most models in use are hybrids where some processes are mechanistically or empirically described (Reckhow and Chapra, 1999).



## 3 REVIEWS OF MECHANISTIC MODELS IN THE EVERGLADES

In this section, the review of mechanistic biogeochemical models is primarily focused on applications in the Everglades. However, we also include several examples that have not been directly applied to the Everglades, but have contributed to the mechanistic biogeochemical modeling studies for the Everglades. A synthesized review of these modeling efforts will be useful to develop more advanced mechanistic biogeochemical models in the Everglades.

### 3.1 Mercury

The Everglades Mercury Cycling Model (E-MCM; Harris et al., 2003) was the first detailed mechanistic model to describe the Hg cycling in the Everglades marsh. This model is based on the mass balance approach, and can predict time-dependent concentrations for three forms of Hg: inorganic, methyl, and elemental. The model divides the natural system into four compartments: the water column, macrophytes, four sediment layers, and a food web (Figure 3). The food web consists of fish, zooplankton, phytoplankton, periphyton, detritus, shrimp, and benthos. The E-MCM was initially calibrated using two years of data (1996–1998) from WCA-3A-15, and subsequently applied to predict the response of fish mercury concentrations to the altered

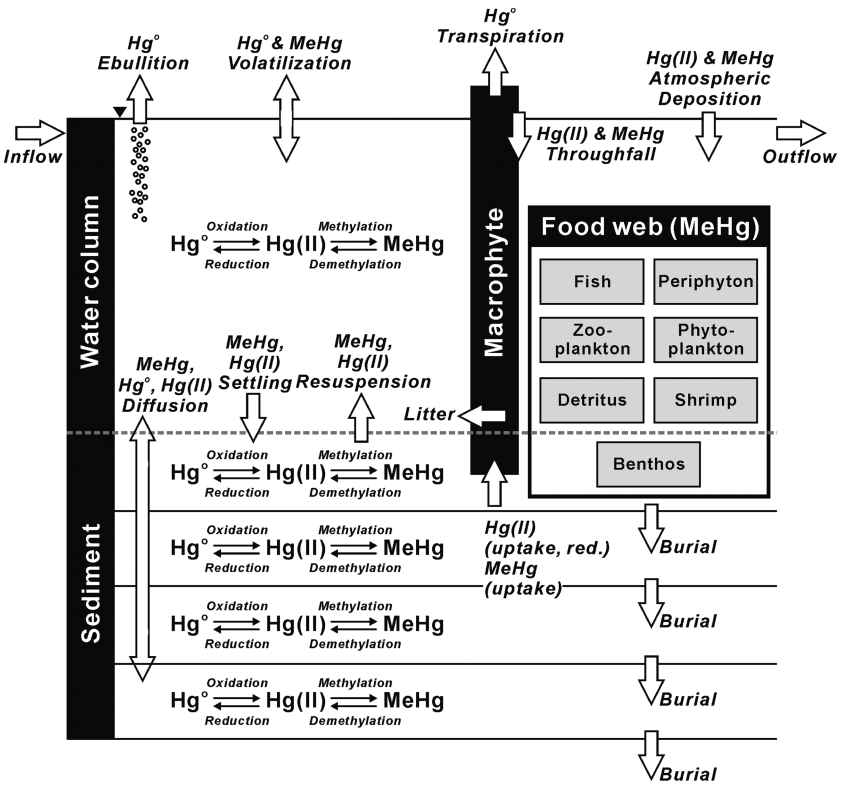


**FIGURE 3.** Hg cycling in E-MCM.

atmospheric Hg deposition (Harris et al., 2000). The E-MCM was further modified to allow multiple cell simulations to be linked in series, with a direct link of an individual cell to adjacent cells immediately upstream and downstream. The modified version was used for transient model calibrations to four individual sites of the Everglades: the Everglades Nutrient Removal (ENR) Project, WCA-2A (F1 and U3), and STA-2 (Harris et al., 2003). The model calibrations were performed against the observed mean concentrations of Hg level in fish as well as inorganic Hg and methyl Hg in surface water. In addition, several simulations of management scenarios were conducted to evaluate the potential effects of changes to flow rates, atmospheric Hg deposition, methylation rates, and TP across ENR Project and WCA-2A sites. One of these hindcasting model results indicated that changes in atmospheric deposition may account for most of the recent changes in largemouth bass Hg levels in terms of both timing and magnitude of change, although the effects of concomitant shifts due to other environmental variables, such as water column sulfate levels needed further elucidation (Atkeson et al., 2005). These results were predicated on rapid rates of turnover of the pool of Hg (II) that was readily bioavailable in surficial sediments for methylation

(Atkeson et al., 2005) because thin surface sediment layer (3 mm) employed by model fitting caused minimal buffering, leading to rapid response to the loading in water column. Sulfur (S) cycling is one of the primary controlling factors on the net methyl Hg production and bioaccumulation in the Everglades ecosystem (Gilmour et al., 2007). Harris et al. (2003) suggested developing a more sophisticated model that can accommodate the essential features of the S cycle, and work is now in progress to capture the complex interactions between methyl Hg production and the S cycle (Axelrad et al., 2008). In summary, the E-MCM integrated several hydrologic and biogeochemical processes, and its demonstration in the Everglades marsh provided a valuable understanding of some of the processes and governing factors of Hg dynamics for this unique ecosystem.



## 3.2 Phosphorus

### 3.2.1 Models that Couple Simple Hydrology and Simple Biogeochemistry

An empirical mass balance approach based on input-output analysis is the simplest model used to describe phosphorus retention in various wetland systems (Kadlec and Newman, 1992; Kadlec and Wallace, 2009; Reddy et al., 1999). The first-order kinetic model referred to as $k{-}C^*$ model or Vollenweider-type model has been most frequently used to explain exponential decrease of P concentration along the flow direction or compare the efficacy of treatment wetlands (Table 1). This model is based on the assumptions that P removal is directly proportional to the P concentration at a given location and the first-order kinetic constant, $k$, called net uptake coefficient or settling velocity, which lumps all P retention processes occurring in wetlands (Kadlec, 1997). Walker (1995) adapted this approach to provide a design basis for STA construction and management. The model was tested against peat and water column monitoring data from WCA-2A, and successfully applied in designing STAs to achieve average outflow TP concentration of 50 ppb or less. This model was also formulated to predict net phosphorus removal via peat accretion due to settling and burial in proportion to the amount of labile P in storage over a long period of time. The Everglades Phosphorus Gradient Model (EPGM) was developed as an expansion to the design model for STAs that includes mass balances between water column and surface soil (Walker and Kadlec, 1996). The EPGM predicted downstream steady-state flow, water column and soil P levels, and peat accretion rate along the horizontal gradient. The model presumed that soil accretion is the only long-term, sustainable mechanism for P removal. For optimizing treatment wetland design and long-term nutrient management, these empirical (relatively simple P cycling) modeling approaches have been used successfully. However, these models may not be able to predict performance of the treatment wetlands

under varied conditions, such as altered flow and vegetation type and density, because these models are not based on transient flow characteristics and the key model parameter, *k*, is not independent to model input condition such as mass loading rate and retention time distribution (Kadlec, 2000; Wang and Jawitz, 2006).

### 3.2.2 Models that Couple Complex Hydrology and Simple Biogeochemistry

Some P models have adapted an integrated approach coupling simple P transport and cycling with fully or semi-distributed watershed- and wetland-scale models (Table 1). The watershed models include AnnAGNPS (Bingner and Theurer, 2009), HSPF (Bicknell et al., 1997), MIKE-SHE (Refsgaard and Storm, 1995), SWAT (Arnold et al., 1994; Neitsch et al., 2002), SWMM (Huber and Dickinson, 1988), and WAM (Soil and Water Engineering Technology [SWET], 2006). These watershed-scale models implement a variety of hydrologic and hydraulic and biogeochemical components, ranging from empirical to physically based approaches (Borah and Bera, 2003; Migliaccio and Srivastava, 2007), primarily to simulate nonpoint source pollution in various watersheds (see Borah and Bera [2004] and their references for the summary of each model application and the details, respectively), including agricultural and urban watersheds in Florida. Several forms of P (dissolved or particulate phases) are simulated with water and sediment flux generated via overland, channel, or groundwater flow and the loss and retention functions are in most cases simply implemented into the models during the flow routings in a watershed based on the land use types (e.g., the wetlands function of WAM; SWET, 2006).

In addition to the watershed-scale coupling, simplified P dynamics have been linked to wetland-scale flow dynamic models (Kazezyilmaz-Alhan et al., 2007; Raghunathan et al., 2001; Tsanis et al., 1998). For example, Tsanis et al. (1998) developed a two-dimensional depth-averaged hydrodynamic/mass transport model with a Vollenweider-type P loss term (sedimentation rate coefficient; 0.03 $day^{-1}$) to simulate water column TP behavior in Cootes Paradise marsh, Canada, and the model predicted TP concentrations reasonably well, both for an overall average of the entire marsh and for individual sites. Similarly, Raghunathan et al. (2001) used Everglades Water Quality Model (EWQM) to describe water column TP transport and retention in the Everglades and test the effects of nutrient reduction scenarios in support of Everglades restoration. The model coupled a spatially distributed, regional-scale flow model (SFWMM) with a P mass balance model that used a simple, apparent net settling rate coefficient that integrated the effects of chemical, biological, and physical processes in each model grid element. The spatially different coefficients (7–11 m/year) were determined through model calibration against data collected in the WCAs and the Everglades National Park. The calibrated model was used to explore the fate and behavior

of water column TP in the Everglades with respect to several hypothetical conditions (no settling, varied atmospheric deposition, and controlled upstream P loads). Hydrologic complexity was sufficiently captured with a two-dimensional model grid in these models; however, the biogeochemistry was represented too simply to describe and simulate details of most internal P cycling processes in wetlands, which have been traditionally regarded as a black box.

### 3.2.3 Models that Couple Complex Hydrology and Complex Biogeochemistry: Midwest, USA

A variety of mechanistic wetland P models have been used to simulate P cycling linked with hydrology submodels (Kadlec and Hammer, 1988; Mitsch and Reeder, 1991; Wang and Mitsch, 2000). Mitsch and Reeder (1991) developed a semimechanistic, wetland compartment model to determine the fate and retention of P in a wetland area adjacent to Lake Erie. The P submodel was coupled with the hydrology and primary productivity submodels and included two storages (water column and sediment), which were linked with linear pathways—sedimentation and resuspension. Also, P uptake by macrophytes was assumed to occur in sediments. The single state variable in the hydrologic model was the volume of water in the marsh, which was controlled by water budget components. Through the model simulations for various hydrologic conditions, P retention ranging from 17 to 52% was estimated in the wetland with the highest retention when high inflows were coupled with high lake levels. The model predicted a net P retention rate (net soil accretion) of 2.9 mg P/$m^2$/day, which was mainly due to the active role of plankton to uptake water column P and be ultimately deposited onto the sediment layer (i.e., plankton sedimentation). Wang and Mitsch (2000) used a similar approach with the addition of a sediment submodel to simulate P dynamics in four constructed riparian wetlands at Des Plaines River, northern Illinois. The P submodel had four compartments, including water column TP, bottom detritus TP, active sediment layer TP, and deep sediment layer TP. The detailed ecosystem model was calibrated and validated against field data measured for the period of 1989–1991. TP budgets calculated from the ecosystem P dynamic model results showed that these wetlands entirely retained 85% of the inlet TP. Based on the detailed P fluxes calculated among the compartments, macrophytes had a relatively low effect on net P retention on the whole system (the amount of P taken up by macrophytes from deep sediments—about 74% of inflow—was considerable, but most was later reincorporated into the sediments), but physical sedimentation played a key role for the overall P retention, despite the existence of substantial intrasystem cycling.

### 3.2.4 Models that Couple Complex Hydrology and Complex Biogeochemistry: Everglades, USA

In the Everglades, various levels of flow-coupled mechanistic P models have been developed to describe flow and P movement in STAs (HydroQual, 1997; Jawitz et al., 2008; Min, 2007; Walker and Kadlec, 2005) and the entire Everglades area (Fitz and Sklar, 1999; Fitz and Trimble, 2006). A fairly complex mechanistic biogeochemical model, Wetland Water Quality Model (WWQM) was developed to simulate changes in wetland water quality (specifically P) under alternative management scenarios, especially in STAs of the Everglades (HydroQual, 1997). WWQM was implemented with mass transport and complex kinetic equations of nutrients in water column, sediment, and emergent vegetation to simulate the P cycling processes. The model first calculated flow dynamics followed by water quality. The flow model was calibrated against data from a prototype STA, the ENR Project (Moustafa and Hamrick, 2000). The structure of the water quality model consisted of four stationary compartments: macrophyte, periphyton, aerobic sediment, and anaerobic sediment. The complexity of the biogeochemical processes included in this model (over 200 parameters) translated to difficult calibration, so the model has not been adopted for management purposes.

Walker and Kadlec (2005) extended their previous models to a DMSTA that enabled simulating transient flow conditions to account for event-driven performance in treatment wetlands with an additional biomass compartment of labile P storage. DMSTA was developed to facilitate the design of STAs to achieve long-term outflow TP concentrations of 10 ppb in the discharges. DMSTA calculates daily water and mass balances in a user-defined series of treatment cells with P cycling parameters. A maximum of six treatment cells can be linked in series or parallel compartments, and each cell is further divided in a series of continuous tank reactors to reflect the residence time distribution. DMSTA considers the biomass component, which is primarily the wetland vegetation that includes three categories: emergent macrophytes, submerged aquatic vegetation, and periphyton. P cycling model parameters, which account for uptake and release from biomass and burial of stable P residuals, were obtained from several wetland systems in the Everglades. The model has been used in several feasibility and design studies of STAs (Burns and McDonnell, 2003) and storage reservoirs (Black and Veatch, 2006) as part of the CERP and regularly updated by calibrating and validating with additional data from full-scale STA treatment cells and other wetlands/reservoirs in the Everglades (Walker and Kadlec, 2005).

Also, a spatially explicit, mechanistic model that targeted prediction of flow and P movement across the South Florida landscape, ELM, was developed (Fitz and Sklar, 1999; Fitz and Trimble, 2006). The landscape model was primarily designed to evaluate the ecosystem responses to alternative water and nutrient management scenarios, and has been applied in the

Everglades restoration efforts. ELM dynamically integrates hydrology, water quality, soils, periphyton, and vegetation, and simulates the hydroecological processes at scales suitable for regional assessment. In addition to the horizontal (2-D) transport of water and constituents, the vertical solutions of the landscape simulation (different ecological processes based on landscape pattern) are calculated in each homogeneous grid cell, known as unit General Ecosystem Model (Fitz et al., 1996). To describe P cycling over each raster grid cell, the model includes four stationary state variables—macrophytes, periphyton, floc, and soil—and several processes including uptake by macrophyte and periphyton, mineralization, sorption, diffusion, and organic soil accretion. ELM does not simulate the flow at hydraulic structures, and thus it imports boundary condition hydrologic data from the SFWMM. The general limitations of this model are high computational demand and extensive data requirement in support of the model development and calibration and validation because of the complex P cycling processes combined with the large number of fully distributed grid cells.



## 4 CASE STUDIES

Case study simulations are described here for two treatment cells from two of the six STAs: STA-1W Cell 4 and STA-5 Cell 1A (Figure 2). Cell 4 in STA-1W (effective area: 1.45 $km^2$), dominated by submerged aquatic vegetation (SAV), is one of the most intensively studied areas due to the relatively longer operational history (DB Environmental Laboratories, 2000, 2002; Dierberg et al., 2002; Dierberg et al., 2005). On the other hand, Cell 1A in STA-5 (effective area: 3.38 $km^2$), dominated by emergent aquatic vegetation (EAV), has been considered one of the challenged systems in STAs in terms of historical TP removal rate (Juston and DeBusk, 2006). Detailed information on the operation and management as well as the physical features of these treatment cells are available in the STA performance chapters of the South Florida Environmental Report annually published by the South Florida Water Management District (SFWMD; Pietro et al., 2008).

Mechanistic P models reviewed in the following two cases show different level of complexity but both were linked to two-dimensional, spatially distributed, flow dynamic and transport models and tested against water column and soil TP data. Flow-coupled mechanistic P models need large amounts of data for model setup, calibration, and validation, as noted by Robson et al. (2008). Time series data including rainfall, evapotranspiration, water level and flow, and water column P concentrations were obtained from the SFWMD online database, DBHYDRO (http://www.sfwmd.gov/org/ema/dbhydro/). For spatially distributed data, including bathymetry, biomass, and floc/soil P, field survey data were interpolated or literature values from either the STAs or the WCA-2A eutrophic area were used for model

initial condition setting. Weekly or biweekly grab sample data of TP concentrations at each inflow structure were used as a transient input source.

In this study, percent model error (PME)—defined as root mean square error (RMSE) divided by the range of the measured data—was used for the model accuracy assessment in addition to RMSE. The PME allows direct comparison between model applications with different output metric ranges, such as in the case studies here where output TP levels measured in STA-5 Cell 1A were generally three times higher than those in STA-1W Cell 4. The model performance in predicting the outlet TP concentration is compared for the two case studies to investigate whether increased process complexity (including additional model compartmentalization, more state variables, and more parameters) guarantees better simulation results.



## 4.1 STA-1W Cell 4 P Dynamics Model

### 4.1.1 Model Setup

For Cell 4 in STA-1W, the modeling framework was the Regional Simulation Model (RSM) developed by SFWMD (2005). The Hydrologic Simulation Engine (RSM-HSE) was used to simulate the flow dynamics and internally coupled with the Water Quality Engine (RSM-WQ) to simulate the transport and reaction dynamics (James and Jawitz, 2007). The model domain consisted of 298 unstructured triangular meshes (average area: 5,100 $m^2$), and the mesh density was further refined in some specific areas to better represent the location of flow structures. The model was calibrated with the water column P data from 1995 to 1998 (4 years) and validated against data from 1999 to 2000 (2 years). The simulation time step of 1 hr was selected considering numerical stability of the hydrodynamic model.

### 4.1.2 P Cycling

This case study evaluated the credibility of a partially lumped mechanistic model in predicting outlet TP levels. Figure 4a illustrates a conceptual model of P cycling that was implemented to simulate the water column, biomass, and soil TP in Cell 4 of STA-1W. The model consists of three state variables and seven kinetic processes. The biomass store includes the combination of several variables such as variety of organisms and plant species. Only the water column TP was considered as a mobile component, whereas the other two state variables were assigned to be stabile (nonmobile). Each kinetic pathway among the stores was modeled with a first-order rate constant.

### 4.1.3 Outflow TP Prediction

Long-term measurements of TP concentrations from 1995 to 2000 at the wetland outflow structure provided an excellent dataset for model calibration and validation. The model calibration was performed by trial and error for a 4-year period (1/10/1995–12/31/1998) by adjusting model parameters

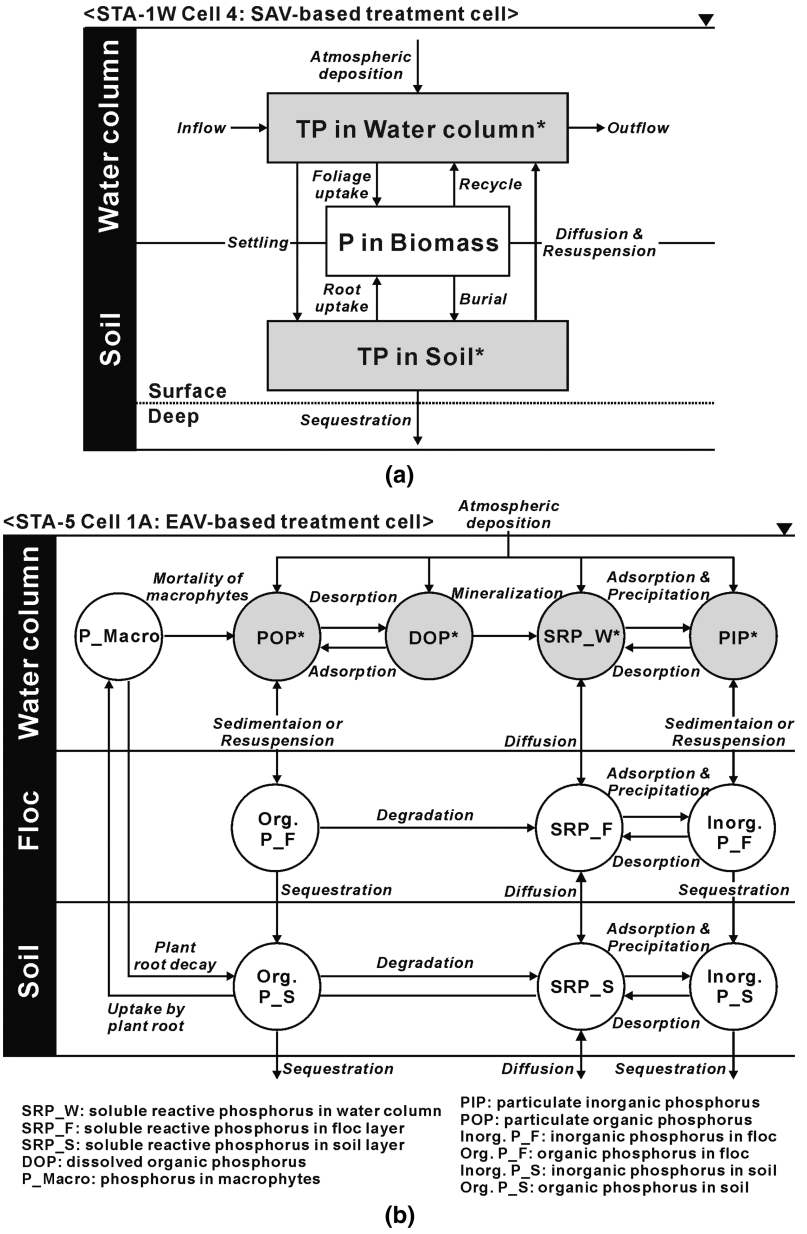


**FIGURE 4.** Mechanistic P cycling applied to case study areas: (a) STA-1W Cell 4 and (b) STA-5 Cell 1A. The state variables denoted with asterisks were compared to the observed time series data.

until optimal goodness of fit metrics were obtained. Figure 5 shows snapshots (March 14, 2000) of the 2-D distribution of water column and soil TP. High concentrations of water column and soil TP along the inflow structures of the northern area, and short-circuiting flow zone along the

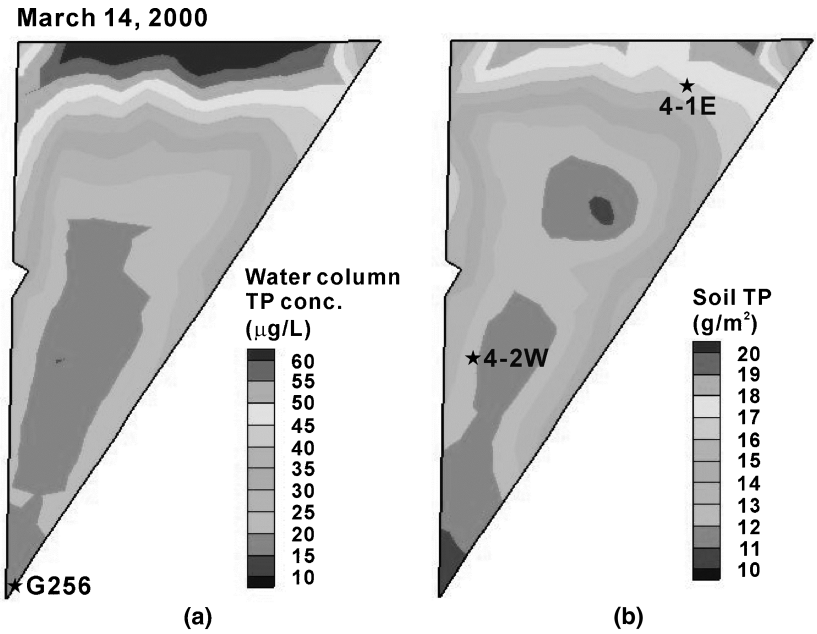


**FIGURE 5.** Snapshots of TP distribution simulated at STA-1W Cell 4 on March 14, 2000. (a) water column TP and (b) soil TP concentrations. Asterisks denote the location of monitoring stations on water column (G256) and soil TP (4-1E and 4-2W).

eastern and western levees (Dierberg et al., 2005) were simulated appropriately (Figure 5). The model predictions corresponded also to the temporal variation of water column TP levels measured at the outlet hydraulic structure, G256 (Figure 6). Comparison between the simulated and observed TP

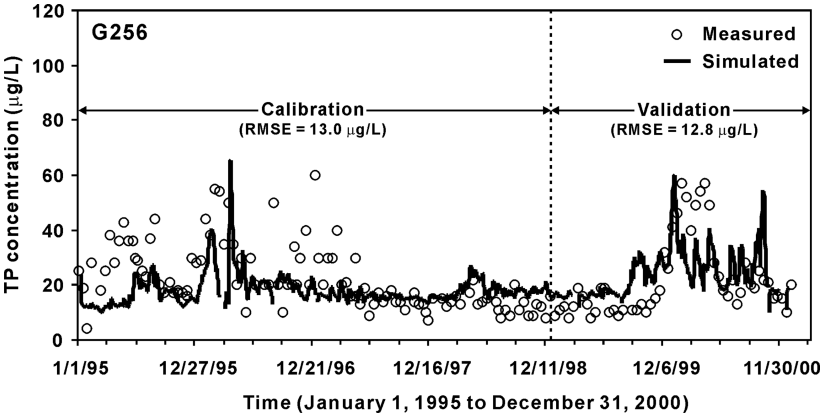


**FIGURE 6.** Measured and simulated TP concentrations at the outflow structure (G256) of Cell 4 in STA-1W for the model calibration period (January 10, 1995–December 31, 1998) and validation period (January 1, 1999–December 31, 2000).

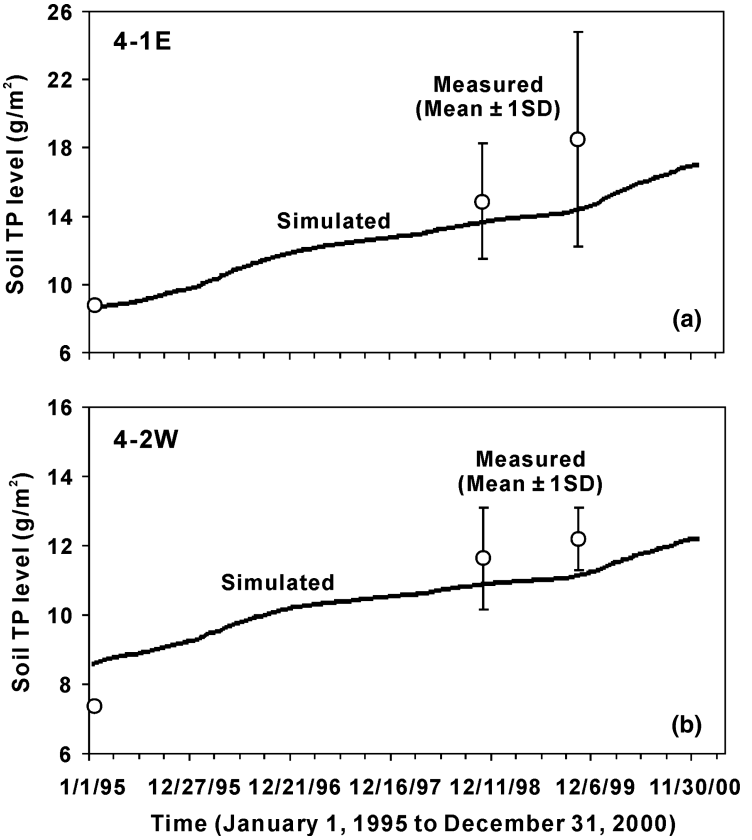


**FIGURE 7.** Measured and predicted soil TP levels at two locations within the Cell 4 of STA-1W. (a) upstream area, 4-1E and (b) downstream area, 4-2W.

concentrations during the model calibration period shows fair agreement (RMSE = 13.0 $\mu$g/L; PME = 23%). Potential sources of the prediction errors include uncertainties in the observed data, and mesh resolution, which was not fine enough to capture high-resolution spatial variations in topography and vegetative distribution. The model validation with independent two year monitoring data (1/1/1999–12/31/2000) resulted in a similar prediction accuracy compared to observed values (RMSE = 12.8 $\mu$g/L; PME = 26%).

Time series profiles of soil TP level simulated at two monitoring stations (4-1E and 4-2W) within Cell 4 (see the locations in Figure 5) are shown in Figure 7. These results show that the model was able to reproduce the spatiotemporal variations of soil TP level over a 5-year period. It is emphasized that even though the simulations did not fully capture all of the short-term variability in water column TP, the overall trend was captured and this allowed good prediction of the more integral effect of P accumulation in the soil. Sensitivity analyses indicated that the outlet TP concentrations were

highly sensitive to changes in settling and release rate constants compared to other P cycling rate constants.

## 4.2 STA-5 Cell 1A P Dynamics Model

### 4.2.1 Model Setup

For Cell 1A in STA-5, the modeling framework was MIKE 21 developed by the Danish Hydraulic Institute (2004). The Hydrodynamics (HD) and Advection-Dispersion (AD) modules were used to simulate the flow dynamics and solute transport, which integrated with Water Quality module (ECO Lab) to simulate the P dynamics. The model consisted of 408 rectangular grids (100 × 100 m), and incorporated time-varying, daily-based measurements of water budget components, such as stage, flow, precipitation, and ET. Monthly averaged net groundwater seepage was determined by minimizing the monthly water budget error. In this model, groundwater as well as surface water flows through hydraulic structures are described as point sources and sinks. An ECO Lab P dynamics model, linked with the HD and AD modules pretested against contemporary water level and chloride concentration profiles at the study area (Min, 2007), was calibrated with the measured water column P data (SRP, DOP, and PP) from May 1, 2003 to April 30, 2004 (1 year) and validated against data from May 1, 2004 to December 31, 2004 (0.67 years). The simulation time step was 10 min.

### 4.2.2 P Cycling

This case study evaluated the credibility of a more complex mechanistic model in predicting outlet TP levels. Figure 4b illustrates a conceptual P cycle that was implemented for Cell 1A of STA-5. The model consists of 11 state variables, 30 processes, 50 constants, and 3 forcing functions. Of the state variables, only four P species in the water column are mobile components and the other variables were fixed at each grid cell. For most of the transformation processes, first-order kinetics formulation was used with the Monod equation incorporated for the growth of macrophytes representing the dominant EAV species found in the cell (*Typha* spp. and *Ludwigia* spp.). In this conceptual model, P dynamics in the floc layer were assumed to play a critical role in regulating the level of P species in the water column. One of the major standing stocks in the wetland ecosystems, phytoplankton and periphyton, were not considered because these components were found to be sparse in eutrophic water samples collected from the northern Everglades (McCormick et al., 1998). All the coupled ordinary differential equations were solved numerically with the Euler method. Daily averaged summation of simulation results on four state variables (SRP_W + DOP + PIP + POP = TP) were compared to the time series TP observations.

### 4.2.3 Outflow TP Prediction

The constants in most kinetic pathways were initially selected based on literature data and finally determined by model calibration on 18 constants. Floc, soil, and biomass-related parameters were first estimated through model calibration by maintaining their dynamic equilibrium condition in the state variables because no time series measurement data for these state variables were available. This calibration approach was based on an assumption of only gradual annual changes in the standing stocks. Model calibration on the parameters related to water column processes was not finalized until the overall simulation error (RMSE) on the model fit of SRP_W, DOP, and PP was minimized. Figure 8 shows the model calibration and validation results of TP at two downstream monitoring stations, G343B and G343C. The model showed a reasonable agreement with spatiotemporal variation of TP concentration profiles. The average RMSE values were 30 and 27 $\mu$g/L during the model calibration and validation period, respectively. These corresponded to the PME of about 17–21%, which were slightly smaller than the values calculated for STA-1W Cell 4. The most sensitive model parameters on SRP_W were the constants regulating EAV dynamics, such as maximum growth rate, uptake half saturation, and macrophyte decay rate constant, as well as adsorption rate constant in the water column. In contrast, the parameters that most directly affected DOP and PP were primarily related to physical processes in water column, including critical flow velocity and POP deposition rate constant (Min, 2007).

## 5 DISCUSSION AND SUMMARY

### 5.1 Level of Complexity in Mechanistic Biogeochemical Models

The previous two case study simulation results on each outlet time series TP data revealed that the mechanistic biogeochemical model with more complexity (Figure 4b) did not guarantee significantly better simulation accuracy compared to the one with less complexity (Figure 4a). Hence, it can be said that the simple mechanistic model is more efficient than the complex one if the ultimate modeling goal is just to predict time series TP concentration profiles at some outlet points.

However, the more complex mechanistic model can provide some insight on the internal processes that the simpler model cannot provide. Figure 9 shows the relative portion of water column P species (SRP, DOP, and PP) to the model prediction error of time series TP level at one of the outlet monitoring stations (G343B) in STA-5 Cell 1A. The model error was defined as deviation of simulated from measured concentration at each time step. Hence, if the error ($C_s - C_m$) was greater than zero, the model prediction was overestimated and if less than zero, the simulation was underestimated.

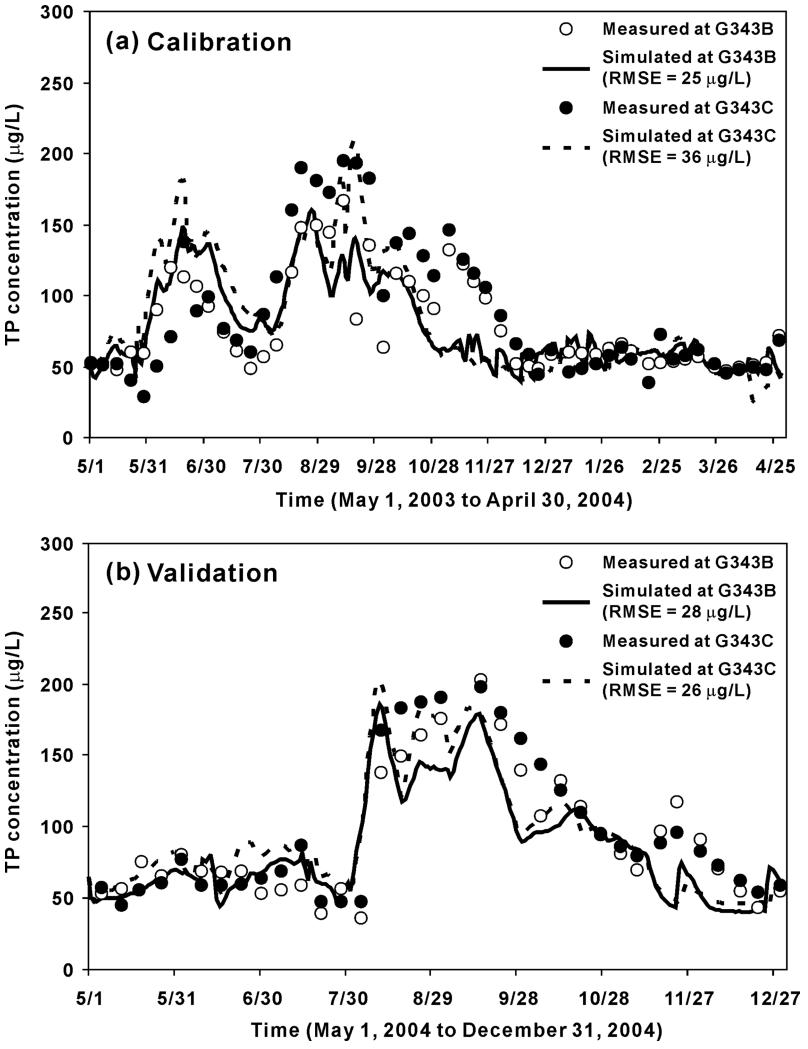


**FIGURE 8.** Measured and simulated TP concentrations at the outflow structures (G343B and G343C) of Cell 1A in STA-5. (a) model calibration (May 1, 2003–April 30, 2004) and (b) validation (May 1, 2004–December 31, 2004).

The annual fluctuation of TP simulation error is closer to the pattern of SRP than those of DOP and PP (Figure 9). This shows that the SRP simulation error generated the largest simulation uncertainty in the TP outlet prediction ($R^2 = 0.69$). The SRP simulation error may be related to biomass (SAV and periphyton) activities that were not fully reflected in the model. The overall overestimation of SRP during the vegetation growth period was likely related to the active growth of unaccounted vegetation. It is expected that incorporating improved understanding (and associated data) for SRP cycling between the water column and biomass into the conceptual model for this

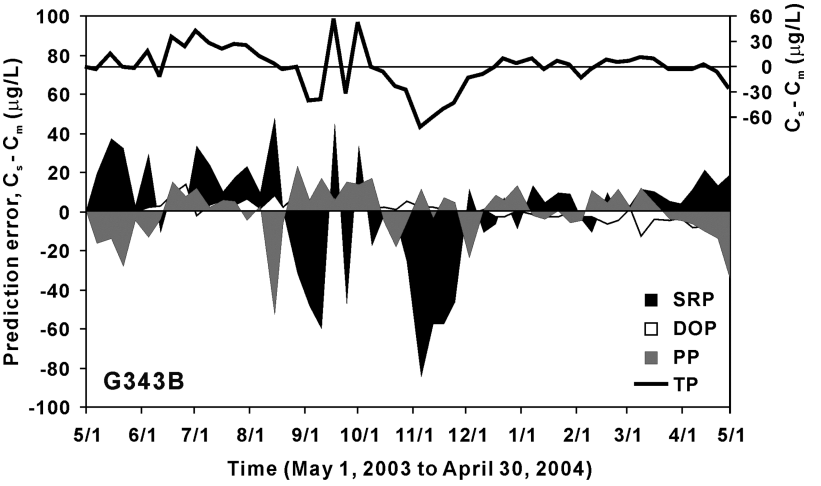


**FIGURE 9.** Model prediction error for TP components (SRP, DOP, and PP) at outlet monitoring station G343B in STA-5 Cell 1A.



treatment cell would result in enhanced model predictive capability on the time series outlet TP level.

Reconciling the tradeoffs in the level of complexity is a continuing challenge for mechanistic biogeochemical models. Some investigators claim that simple models (closer to empirical approach) have better practical value (Kadlec and Wallace, 2009; Wong et al., 2006) because no mechanistic models are able to explain the infinite complexity of the underlying phenomena, and that significant uncertainties are introduced in estimating a large number of model parameters. Others emphasize that more complex mechanistic models have robust theoretical basis and thus better predictive potential (Fitz et al., 2003; Jawitz et al., 2008; Robson et al., 2008). According to the model categories suggested in this paper, the former may prefer the simple biogeochemical modeling approaches coupled to simple or complex hydrology (Sections 3.2.1 and 3.2.2), while the latter may prefer the complex biogeochemical modeling approaches based on complex flow models (Sections 3.2.3 and 3.2.4). However, it is noteworthy that all useful models involve an element of empiricism where some processes are empirically described in a broad aspect (Reckhow and Chapra, 1999). In this respect, most of the P models applied in the Everglades wetland (Table 1) can be considered hybrids between mechanistic and empirical models.

What level of complexity is warranted in mechanistic biogeochemical models to be used in support of the Everglades restoration? To address this dilemma, first we may need to answer what kind of predictions are desired or what hypotheses can be tested through a modeling study. For example, what if the external load of TP is increased to a specific location in the Everglades due to increased flow as a result of hydrologic restoration? Or

how much P internal loading is expected at some P-enriched soil areas like WCA-2A if a significant reduction of external TP loading is maintained in the future as a result of reduced P export from upstream areas? Hence, the appropriate level of complexity of a mechanistic biogeochemical model is highly dependent on the specific modeling objectives. For the case study examples, if the modeling interest were to simulate the behavior of soluble and particulate P species in STAs independently, the relatively simple P cycling model described in Figure 4a may not be sufficient to fulfill the modeling goal. In contrast, if the modeling target was only to simulate the outlet TP concentration profile, a simpler P cycling model than Figure 4a may be enough to meet the need. Next, we may also need to decide the model utility: long-term management purpose (close to the style of DMSTA), or scientific investigation for better process understanding among the ecosystem compartments (close to the style of ELM). Finally, the level of complexity is definitely limited by data quality collected from field and laboratory. Therefore, each process complexity should be represented appropriately based on the specific modeling objectives, the model utility, and the availability of spatiotemporal data.

Constructing a mechanistic model is to mirror the complexity of the natural system (Arhonditsis et al., 2006; e.g., complex interactions of hydrologic and biogeochemical processes in wetland systems). It is unlikely that even an extremely complex mechanistic model can mimic the reality of the natural system. Therefore, regarding the level of complexity of flow-integrated, mechanistic biogeochemical models to be used effectively for Everglades restoration, we suggest developing a hybrid model where some processes are empirically lumped and others are mechanistically represented on the basis of the model goal and data availability. The determination of optimal aggregation level of processes is challenging. This may be determined with a rigorous testing of the model with different combination of aggregations. In this paper, our goal was not to suggest what complexity of the integrated model is optimal, but rather it was to show the suitability of different complexity of biogeochemical models with available existing knowledge and data.



## 5.2 Mechanistic Modeling Needs for Everglades Restoration

One of the most important features of a model is the predictive capability. From this view, a mechanistic biogeochemical model with intermediate level of complexity that straddles oversimplification and overparameterization is preferred because it both promotes better biogeochemical process understanding in a system and provides a process-based data integration tool. Also, it allows delineating a cause and effect relationship within a model efficiently and predicting the response of a target ecosystem component to some changes in other state variables or environmental factors.

In addition, a mechanistic biogeochemical model for Everglades restoration should be based on a spatially distributed flow dynamic modeling approach because hydrology is the most critical factor sustaining the structure and function of wetland ecosystems. The importance of hydrology on biogeochemical dynamics has been well acknowledged in the Everglades marsh (Noe and Childers, 2007), as it provides the basis for horizontal and vertical transport processes, and biogeochemical transformations of nutrients in surface water and upper sediment. Also, flow-integrated mechanistic biogeochemical modeling can provide a guideline for optimized hydrologic restoration through testing scenarios on the future impact of restored hydrology on the wetland ecosystem, maximizing the beneficial restoration impacts and minimizing the side effects.

The following scientific research needs are identified for improved development of a conceptual model that defines key interactions among the ecosystem variables in the Everglades. First, the roles of the floc layer, commonly observed in most areas of the Everglades, have been rarely investigated, particularly quantitative mass transport with other key stores, such as water column, soil, and biomass. Second, it is necessary to develop submodels for biomass (EAV, SAV, and periphyton) dynamics, which are calibrated based on time series field and laboratory data collected at several locations. These submodels may be linked with complementary models of water column and floc and soil layer processes to approach an ecosystem-level mechanistic biogeochemical cycle. Finally, better integration is warranted between data collection and modeling efforts. Data should be collected based on important processes identified during careful construction of a conceptual model that meets the predictive modeling needs. Similarly, new understanding that evolves from observations and measurements can be used to improve the conceptual model. Such bidirectional feedback between conceptual model development and spatiotemporal monitoring is recommended to facilitate both processes.



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