Phosphorus Biogeochemical Model Complexity and Prediction Performance in a Large South Florida Stormwater Treatment Wetland

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Introduction

Mechanistic (or "process-based") models have been increasingly used in wetlands to assist in understanding the system dynamics and quantify the wetland responses to a variety of changes in order to support the management strategies. A key question, however, is how complex of a biogeochemical model structure is appropriate to make reliable predictions based on the available data and knowledge of the system. Modeling is most effective when the reasons for selection of a given model are clearly understood. Generally, the model structure is formulated based on judgments (which are often implicit) about the process details that need to be considered. Here, we examine five models of varying complexity that describe phosphorus (P) biogeochemical cycling in one of the treatment cells of Stormwater Treatment Area 1 West (STA 1W). The hypothesis evaluated here is that the biogeochemical model prediction accuracy in treatment wetlands is increased as the modeled process complexity increases, but the benefits of increased accuracy are small compared to the costs of added complexity.

Fig. 1. Conceptual illustrations of relation of modeling efforts (i.e., model complexity) to prediction accuracy and model effectiveness

Study Objectives

- To develop five P cycling models in different levels of process complexity (from low-level to high-level mechanistic explanation of P cycling processes), coupled with two-dimensional hydrodynamic model in a Cell 4, STA 1W of northern Everglades.
- To quantify prediction errors for each complexity.
- To evaluate the model complexity and identify the 'best' level of process complexity which is simultaneously optimal for predicting outflow total P concentrations and that balances the benefits of increased efforts that is needed to setup, calibrate and validate the model based on available data.

Study Site

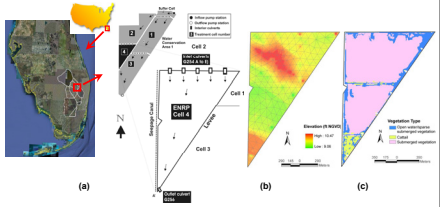

Fig. 2. Study site: (a) location map (b) model mesh and bed elevation (c) vegetation map. The mean bed elevation of raster cells for each mesh element was used.

STA 1W, formerly known as Everglades Nutrient Removal (ENR) Project, is located along the northwestern boundary of Water Conservation Area 1 in central Palm Beach County, Florida. Cell 4 is one of treatment cells of STA 1W which is dominated by submerged aquatic vegetation (SAV) and comprised a total of 147 ha (363 acres) marsh area. The bottom elevation was approximately ranged from 2.7 to 3.2 m (1929NGVD).

Model and Data

Hydrologic Model: Regional Simulation Model (RSM), developed by South Florida Water Management District (SFWMD) (SFWMD, 2005).

- Two-dimensional modeling framework with heterogeneous inputs.

Transport and Reaction Model: Regional Simulation Model-Water Quality (James and Jawitz, 2007).

- Internally coupled with RSM.

- Hydrodynamic calibration: Cell 4 tracer data (Dierberg et al., 2005).
- Validation: Outlet discharge at G256 structure from 1995 to 2000.
- Additional water budget and transport processes validation: Chloride (assumed to be conservative tracer) concentrations at two internal monitoring stations from 1995 to 1999.
- P cycling model calibration/validation: Outflow total P concentrations at G256 structure.

Data:

- The bulk of the field measurement data (hydrological, meteorological and water quality) employed in this study were collected by SFWMD and publicly available on their environmental database, DBHYDRO (http://my.sfwmd.gov/dbhydroplsql/show_dbkey_info.main_menu).
- Atmospheric deposition of total P was based on the study conducted at ENR Site (Ahn and James, 2001).
- Spatial data e.g. topography, vegetation, and initial soil total P were obtained from SFWMD personnel.

Biogeochemical Model Structures

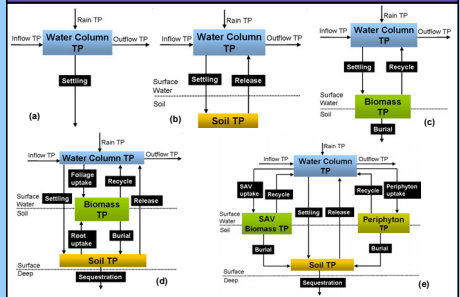

Fig. 3. Phosphorus cycling models with increasing complexity: (a) Model 1 (M1D) - settling rate (b) Model 2 (M2D) - settling and release between water column and soil (c) Model 3 (M3D) - exchange between water column and biomass (DMSTA2; Walker and Kadlec, 2005) (d) Model 4 (M4D)- exchange between water column, soil and biomass (e) Model 5 (M5D) - exchange between water column, soil, SAV and periphyton biomass.

Characterization of Complexity Index

The complexity of the model was determined by using the level of detail in the processes that make up the model (number of calibration parameters/state variables), and spatial descriptions (Costanza and Sklar, 1985).

where C_i = complexity index for mode i (e.g., compartments/parameters and space); K_i = scaling factor for model i which reflects to the relative difficulty in adding processes, and mesh elements in space.

$$C_i = \frac{N_i - 1}{K_i + (N_i - 1)} x100$$

Characterization of Prediction Accuracy

- Prediction accuracy index was determined based on the deviation between model simulated values and observed data (i.e., modeling error).
- Two types of objective functions were used to estimate modeling error:
  - Root Mean Square Error (RMSE)

$$E_{1,k} = \sqrt{\frac{1}{n_k}\sum_{i=1}^{n_k}(S_{i,k} - O_{i,k})^2}$$

  - Mean Absolute Error (MAE)

$$E_{2,k} = \frac{1}{n_k}\sum_{i=1}^{n_k}\left|S_{i,k} - O_{i,k}\right|$$

$$E_{t,m} = \frac{1}{2}\left[\frac{m_k}{\sum_{k=1} max(E_{1,k})} + \frac{m_k}{\sum_{k=1} max(E_{2,k})}\right]$$

$$\phi_m = 1 - E_{t,m}$$

where S and O, simulated and observed values for each sampling event i; k, model application mode (i.e., calibration, validation 1, and validation 2); n_k, total number of observations for each mode k; $E_{t,m}$, total mean normalized error for each model m; m_k, application mode for each model m; ϕ_m, prediction accuracy index for each model m.

Model Effectiveness

The best model is the one that describes accuracy of model prediction in relation to the efforts needed to develop the model. To determine the rank of the model, we developed an index of model effectiveness. The index was calculated as the "coefficient of effectiveness" for each model by normalizing the prediction accuracy with complexity index.

where ε_m, coefficient of effectiveness for each model m; and C_m, complexity index (i.e., modeling efforts) for each model m.

$$\varepsilon_m = \frac{\phi_m}{C_m} x100$$

Results

- Models generally capture the temporal variation of outflow total P concentrations in Cell 4, STA 1W (*Fig. 4*).
- Model performance statistics (RMSE and MAE) are based on outflow total P concentrations at G256 structures (*Table 1*).
- The prediction accuracy for Model 3 (M3D) was higher compared to other models. M3D uses second-order, non-linear settling and recycle processes (Walker and Kadlec, 2005)
- Simulating biomass P in two compartments (i.e. SAV P and periphyton P), using Monod-type equation for growth of vegetation did not improve the prediction results compared to first-order processes between water column, soil and biomass (M4D).

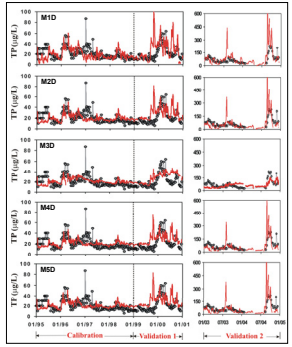

Fig. 4. Observed and simulated outflow total phosphorus concentrations for five biogeochemical models under calibration and validation periods

Results (contd.)

*Table 1: Assessment of simulations of outflow total phosphorus concentrations (Note: *Validation 2 includes period of two major hurricanes (i.e., Frances and Jeanne))*

Model Type	ID	Calibration		Validation 1		Validation 2*	
		Jan 1995 - Dec 1998		Jan 1999 - Dec 2000		Jan 2003 - Dec 2004	
		RMSE (µg/L)	MAE (µg/L)	RMSE (µg/L)	MAE (µg/L)	RMSE (µg/L)	MAE (µg/L)
Model 1	M1D	12.3	9.0	21.5	14.4	119.8	54.5
Model 2	M2D	10.3	7.7	16.8	12.6	96.3	44.8
Model 3	M3D	9.6	7.4	13.4	11.4	46.8	36.5
Model 4	M4D	9.7	7.4	15.7	12.4	87.8	41.8
Model 5	M5D	9.9	7.7	17.1	13.0	99.8	46.9

Table 2: Assessment of complexity index, prediction accuracy and effectiveness

Model Type	C_c	C_s	C_m	$E_{t,m}$	ϕ_m	ε_m
M1D	2	16.5	9.3	0.93	0.07	0.8
M2D	7.4	16.5	12.0	0.77	0.23	1.9
M3D	12.3	16.5	14.4	0.63	0.37	2.6
M4D	16.7	16.5	16.6	0.73	0.27	1.6
M5D	20	16.5	18.3	0.78	0.22	1.2

C_c = complexity index for biogeochemical process descriptions; C_s = complexity index for spatial descriptions, which is used constant because same spatial complexity was used for each model.

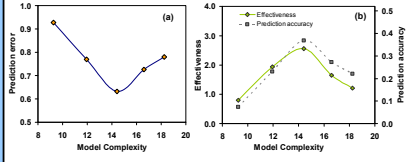

Fig. 5. Effects of model complexity on (a) prediction error and (b) accuracy and effectiveness

Conclusion and Future Works

- Results show that there is trade-off between appropriate level of process-complexity and prediction accuracy. As the model becomes more complex in terms of adding state variables/parameters, prediction accuracy is initially increased but lowered for more complex models.
- It appears that there is an optimum complexity beyond which benefits of increasing process complexity is less effective.
- Future work involves developing five additional spatially lumped models with biogeochemical model structures discussed above, and evaluating model effectiveness using additional criteria (such as model power).

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