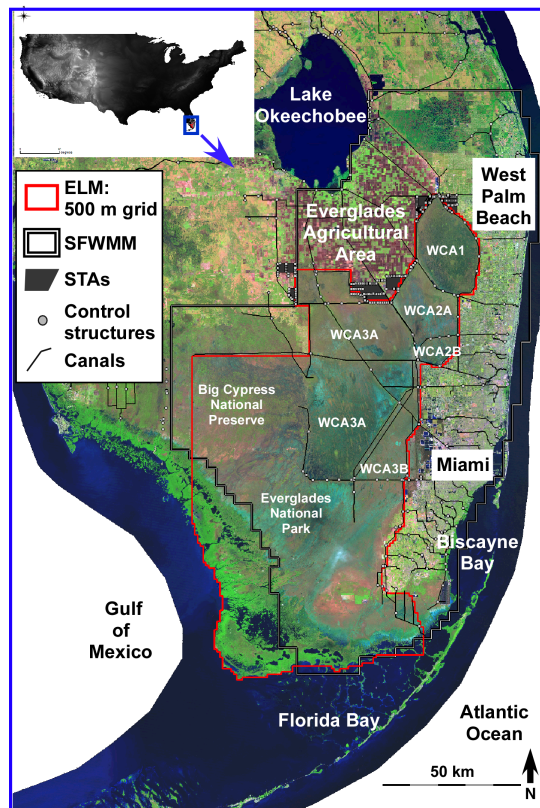


Documentation of the Everglades Landscape Model: ELM v2.8.6 - **Sulfate** Module



<http://ecolandmod.ifas.ufl.edu>

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Preface

Documentation purpose

This report documents the update of the Everglades Landscape Model (ELM) from v2.8.4 to v2.8.6 with a new **sulfate** module, and includes information on *supporting data, algorithms, and performance*. This document and further supporting information are maintained on the EcoLandMod web site:

<http://ecolandmod.ifas.ufl.edu>

We describe the code and data associated with the **sulfate water quality history-matching model performance** of the regional ELM v2.8.6, the version which is being used in to evaluate sulfate water quality responses to management alternatives for the Comprehensive Everglades Restoration Plan's Aquifer Storage and Recovery Project. (ASR) The results of that ELM application are to be contained in a separate documentation report that is specific to that project, to be available on the EcoLandMod web site.

This is a **documentation update, limited to describing changes that were made in model design and data during the transition from ELM v2.8.4 to ELM v2.8.6¹**. A number of original ELM v2.5 and v2.8.4 Documentation Chapters are not included here, as their content remains unchanged; those reports are also available at the EcoLandMod web site.

The only **three Chapters** included in this ELM v2.8.6 Documentation Report are those that contain significant new information that is relevant to current application objectives.

Document organization

*(see ELM v2.5) Chapter 1: **Introduction** to the Everglades and the model **Goals & Objectives**.*

*(see ELM v2.5) Chapter 2: General overview of **Wetland Ecological Models**.*

*(see ELM v2.5) Chapter 3: Graphical and verbal descriptions of the South Florida and General Ecosystem **Conceptual Models** on which the ELM is based.*

- **Chapter 4:** Graphical, verbal, and statistical-summary descriptions all of the updates to **Data** that are used in the new model application.
- **Chapter 5:** Graphical, verbal, and mathematical descriptions of the updates to **Model Structure** and algorithms.
- **Chapter 6:** Analysis of **Model Performance** relative to the historical period of record in the regional system (1981 - 2000).

*(see ELM v2.5) Chapter 7: Aspects of **Uncertainty** in the model and associated data, including sensitivity analysis, appropriate model expectations, and model complexity.*

*(see ELM v2.5) Chapter 8: Descriptions of **Model Application** in the regional Everglades system. NOTE: this v2.5 Chapter is outdated; see EcoLanMod web site for published applications.*

*(see ELM v2.5) Chapter 9: Descriptions of past and planned **Model Refinements**.*

*(see ELM v2.5) Chapter 10: **User's Guide** that provides the simple steps to installing and running this Open Source model.*

¹ The last public release of code and documentation was for ELM v2.8.4.

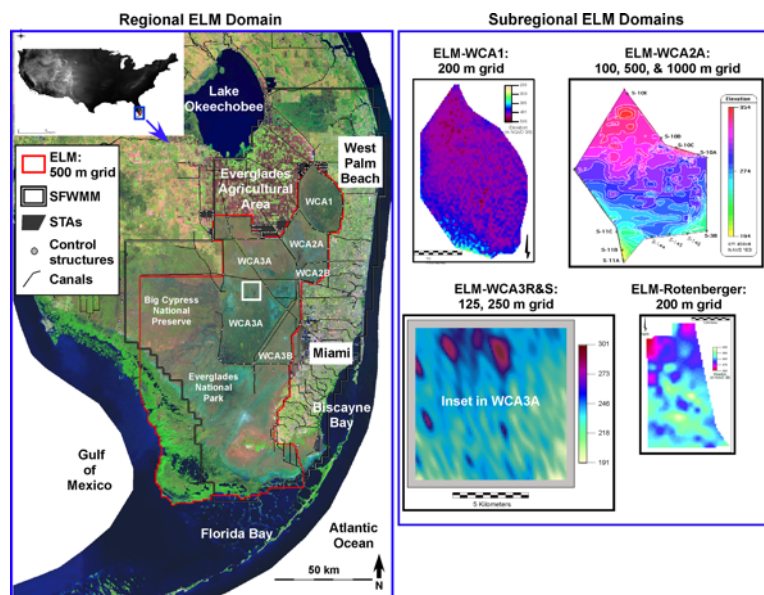
Acknowledgments

Funding for this ELM application update came from the US Army Corps of Engineers. In particular I thank M. Shafer (USACE) for providing the technical guidance in developing the sulfate module for this project, and W. Orem and D. Krabbenhoft (US Geological Survey) for their invaluable expertise that we collaboratively applied towards formulating the sulfate loss algorithms, including their extensive data observations used in the development and refinement of the sulfate module. I also express sincere thanks to the many individuals who have contributed in developing the ELM framework over the years, as cited in prior documentation reports and journal publications.

Executive Summary

Today's Everglades are significantly different from the landscape that existed a century ago. Humans compartmentalized a once-continuous watershed, altering the distribution and timing of water flows, and increasing the quantity of nutrients that move into the Everglades. The result is a degraded mosaic of ecosystems in a region that is highly controlled by water management infrastructure. However, plans are being developed and implemented to restore parts of this system towards their earlier state.

To support scientific evaluations of restoration plans, computer simulation models can be used to predict the relative benefits of one alternative plan over another. One such tool is the Everglades Landscape Model (ELM). The ELM is designed to improve understanding of the ecology of the Everglades landscape, and can be applied at a range of spatial and temporal scales depending on the project requirements. This model integrates, or dynamically combines, the hydrology, water quality, and biology of the mosaic of habitats in the Everglades landscape. It is a state-of-the-art *model that is capable of evaluating long-term benefits of alternative project plans with respect to hydrology, water quality and other ecological Performance Measures.*



Existing regional and subregional applications of the ELM, including the 500 m grid resolution application developed for the regional Everglades system.

Because the ELM was designed to be explicitly scalable, it is relatively simple to adapt (spatial input map) data to accommodate the scientific objectives that may call for a particular scale of grid resolution or extent. For v2.8² of the model, we developed a 500 m (vs older 1 km) grid resolution regional application.

Subsequent updates included a variety of enhancements, and this latest *update to ELM v2.8.6 includes a new module to simulate sulfate transport and fate* in the landscape. This Documentation Report update is specific to the sulfate module, and includes the

² The tertiary subversion designation of the first v2.8 public release was v2.8.3.

information necessary for scientists and planners to understand this application of ELM, including *a) the ELM objectives, b) how it works, and c) how well it works.*

The fine spatial scale and very good historical performance of the model may be useful in a variety of projects involving Everglades synthesis and management. Of particular interest with respect to ecological processes and patterns, this scale of ELM hydrologic output exhibited detailed spatial patterns of flow, with improved connectivity among and within habitats (such as sloughs) relative to the 4x (ELM v2.5) or ~40x (SFWMM v5.4) coarser-scale resolution hydrologic models previously available for the greater Everglades region.

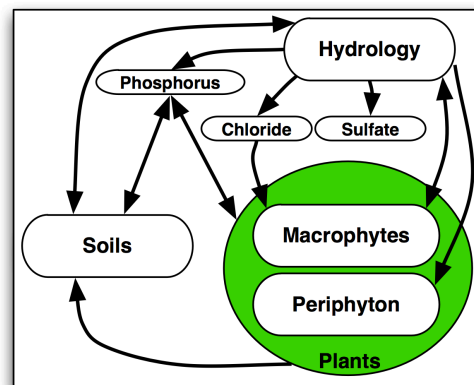
The **new sulfate module demonstrated excellent model "skill"** in hindcasting sulfate concentrations in the regional landscape (median offset, or bias, in marshes was 0 mg l^{-1}), consistent with performance of other ELM water quality modules. We are using this fine-scaled regional application to help evaluate multi-decadal, landscape sulfate water quality responses to future management alternatives for the Comprehensive Everglades Restoration Plan (CERP) Aquifer Storage and Recovery (ASR) project.

Model Goals (see <http://ecolandmod.ifas.ufl.edu/background>)

- Develop a simulation modeling tool for integrated ecological assessment of water management scenarios for Everglades restoration
 - Integrate hydrology, biology, and nutrient cycling in spatially explicit, dynamic simulations
 - Synthesize these interacting hydro-ecological processes at scales appropriate for regional assessments,
 - **Understand and predict the relative responses of the landscape to different water and nutrient management scenarios**
 - Provide a conceptual and quantitative framework for collaborative field research and other modeling efforts

Model Design (see <http://ecolandmod.ifas.ufl.edu/models>)

- Can be applied at multiple spatial or temporal scales, for regional or subregional evaluations
 - Regional application at fine resolution (40x finer than SFWMM³)
 - Multi-decadal (36-yr) simulation period
- Combine physics, chemistry, biology – *interactions*
 - *Hydrology*: overland, groundwater, canal flows
 - *Chloride & sulfate*: transport and fate
 - *Phosphorus*: cycling and transport
 - *Periphyton*: response to nutrients and water
 - *Macrophytes*: response to nutrients, chloride and water
 - *Soils*: response to nutrients and water



³ South Florida Water Management Model, the widely-accepted simulation tool used for regional evaluations of water management alternatives

- Combine ecological research with modeling
 - research advances led to model refinements
 - model output aided research designs

Model Reliability (see <http://ecolandmod.ifas.ufl.edu/publications>)

- Excellent performance (1981 - 2000 history-matching, ELM v2.8.6)
 - *Hydrology*: the offset (median bias) of predicted and observed values of water stage elevations in the marsh was 0 cm
 - *Water quality*: the offset (median bias) of predicted and observed values of phosphorus in the marsh was 0 $\mu\text{g L}^{-1}$; chloride was 8 mg L^{-1} ; **sulfate** was 0 mg L^{-1}
- Tested computer code
 - evaluated model response to wide range of conditions (sensitivity analyses)
 - years of experience in testing and refining code
 - applied at different scales for regional and sub-regional evaluations
- Uses best available data
 - comprehensive, unique summary of Everglades ecology
 - thorough QA/QC of input data
 - continuous interactions with other Everglades scientists and engineers

Model Reviews (see <http://ecolandmod.ifas.ufl.edu/publications>)

- Open Source
 - All ELM data and computer source code freely available on web site
 - Requires only Open Source (free) supporting software
- Publications
 - 1996-2012: Peer-reviewed scientific journals and book chapters
 - 1993-2013: Technical reports published by SFWMD and UF
- CERP⁴ Model Refinement Team
 - 2003: Recommended independent peer review
- Independent Panel of Experts
 - 2006: Peer review of ELM by an independent panel of experts
- CERP Interagency Modeling Center
 - 2007: Review of ELM for CERP applications

Model Application (see <http://ecolandmod.ifas.ufl.edu/projects>)

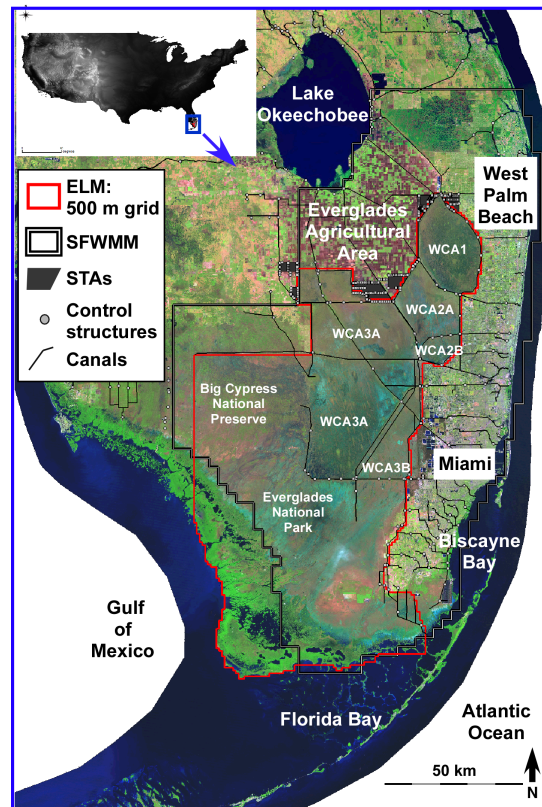
- Specific **model objectives** (Performance Measures, multi-decadal scales)
 - **Fine-scale hydrologic** output for use in “driving” other ecological models
 - **Phosphorus** 1) water column concentrations and 2) accumulation in soils along spatial gradients
 - Other ecological Performance Measures as needed for projects: **soil accretion/loss; vegetation succession; periphyton dynamics; sulfate** dynamics

⁴ Comprehensive Everglades Restoration Plan

- Appropriate interpretation
 - **Relative comparisons** of Performance Measures under scenarios of alternative water management plans, at multi-decadal, landscape scales
- Recent applications
 - ELM v2.8.1 application to large marsh impoundment near **Davis Pond, Louisiana**, 30 m grid resolution; initial application for use in evaluating **landscape evolution scenarios** in a highly managed coastal marsh
 - ELM v2.8.2 application to subregional domain of **Water Conservation Area 1**, 200 m grid resolution; evaluated hydrologic and water quality responses to **simple management & restoration scenarios**
 - ELM v2.8.4 application to **regional Everglades**, 500 m grid resolution; evaluated water quality and other ecological responses to **CERP Decomp project Alternatives**
 - ELM v2.8.4 application to **regional Everglades**, 500 m grid resolution; for **SERES project**, evaluating water quality and other ecological responses to novel CERP project Alternatives
 - ELM v2.8.5 application to **southeast Spain** region, 200 m grid resolution; evaluating **water resource sustainability** in response to land use & climate change
 - ELM v2.8.6 application to **regional Everglades**, 500 m grid resolution; evaluating **sulfate** water quality responses to **CERP ASR project Alternatives**

Documentation of the Everglades Landscape Model: ELM v2.8.6

Chapter 4: Data



<http://ecolandmod.ifas.ufl.edu>

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Chapter 4: Data

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4.1 Overview

The focus of this Chapter is the description of changes to data used in the 500 m resolution regional ELM v2.8.6 application, relative to those documented for the ELM updates from v2.5.2 through v2.8.4.

For this ELM v2.8.6 regional application, we added a new module of sulfate losses from the surface water (see Chapter 5 Model Structure), and that module has no affect on any of the other simulated hydrologic, biogeochemical, or biological dynamics.

The only changes from v2.8.4 to v2.8.6 are the addition of this sulfate (SO₄) module. Thus the only data changes were the additions of sulfate boundary conditions, a net settling rate map, and observed data for use in calibrating the model performance for sulfate concentrations in surface waters. This ELM v2.8.6 Data Chapter thus makes extensive reference to the regional ELM v2.5.2 and v2.8.4 Documentation Reports' Data Chapters, which are available at:

<http://ecolandmod.ifas.ufl.edu/publications>

For reader convenience, several fundamental data components (e.g., model domain map) are copied here from the prior v2.8.4 documentation report. **New sulfate data components are highlighted in red font.**

4.2 Background

4.2.1 Application summary

The U.S. Army Corps of Engineers provided the funding to develop a new ELM module to simulate sulfate (SO_4) loss from the surface water. The only data changes for this new ELM v2.8.6 application involved those associated with sulfate. All of the other data used in this application remain the same as those used in the regional ELM v2.8.4, and thus documentation of those data are found in prior publications: ELM v2.8.4 Documentation Report¹ and the ELM v2.5 Documentation Report².

We will apply this fine-scaled regional application to help evaluate sulfate water quality responses to future management alternatives for the Comprehensive Everglades Restoration Plan (CERP) Aquifer Storage and Recovery (ASR) project. The results of that application will be posted on the EcoLandMod web site.

¹ Fitz, H.C., and R. Paudel. 2012. Documentation of the Everglades Landscape Model: ELM v2.8.4. Ft. Lauderdale Research and Education Center, University of Florida. <http://ecolandmod.ifas.ufl.edu/publications/>. 364 pp.

² Fitz, H.C., and B. Trimble. 2006. Documentation of the Everglades Landscape Model: ELM v2.5. South Florida Water Management District, <http://ecolandmod.ifas.ufl.edu/publications> (Reviewed by independent expert panel, review report at <http://ecolandmod.ifas.ufl.edu/publications>) 664 pages.

4.2.2 Metadata

All of the model input data files (Table 4.1) have basic metadata associated with them.

Type	Input filename	Description
Model domains	ModArea	Define spatial domain
	gridmapping.txt	Link coarse-fine grids
Initial condition maps	icSfWt	Initial surface water
	icUnsat	Initial unsaturated water
	Elevation	Initial land elevation
	Bathymetry	Initial (and constant) creek bathymetry
	soilBD	Initial (and constant) soil bulk density
	soil_orgBD	Initial (and constant) soil organic bulk density
	soilTP	Initial soil phosphorus
	HAB	Initial habitat type
	icMacBio	Initial total macrophyte biomass
Boundary conditions	BoundCond	Grid cells allowing boundary flows
	BoundCond_stage.BIN	Boundary stage/depth time series
	rain.BIN	Rainfall time series
	ETp.BIN	Potential ET time series
	AtmosPdepos	(optional) map, total atmospheric P deposition
	AtmosCLdepos	(optional) map, total atmospheric Cl deposition
	CanalData.struct_wat	Structure: water flow time series
	CanalData.struct_TP	Structure: phosphorus conc. time series
	CanalData.struct_TS	Structure: salt (chloride) conc. time series
	<i>CanalData.struct_SO</i>	<i>Structure: sulfate conc. time series</i>
	CanalData.graph	Recurring annual time series of stage regulation
	Static attributes	CanalData.chan
CanalData.struct		Water control structure attributes
basins		Basin/Indicator Region locations
basinIR		Basin/Indicator Region hierarchy
GlobalParms_NOM		Parameters: global
HabParms_NOM		Parameters: habitat-specific
HydrCond		Parameters: map of hydraulic conductivity
<i>soil_SO4SetVel</i>		<i>Parameters: map of sulfate net settling rate</i>

Table 4.1. List of all of the files that are input to the ELM³, showing the two *new input files in italics*.

³ Two other files, outside of the Project's "Data" directory in the "RunTime" directory, are input to the model and serve to configure the model at runtime. See the User Guide Chapter for information on the "Driver.parm" and "Model.outList" configuration files.

4.3 Model domains

4.3.1 Spatial domain

The ELM can be applied at a variety of grid scale resolutions and extents without changing any source code. For an application at a particular spatial grain and/or extent, the following data files are used to define the model at the desired scale: 1) the appropriate grid resolution/extent of each of the map input files; 2) the grid resolution and geographic (upper left) origin in the two databases that define the canal/levee locations and water control structure attributes; and 3) the linked-list text file that maps coarser-grid data to the selected model application.

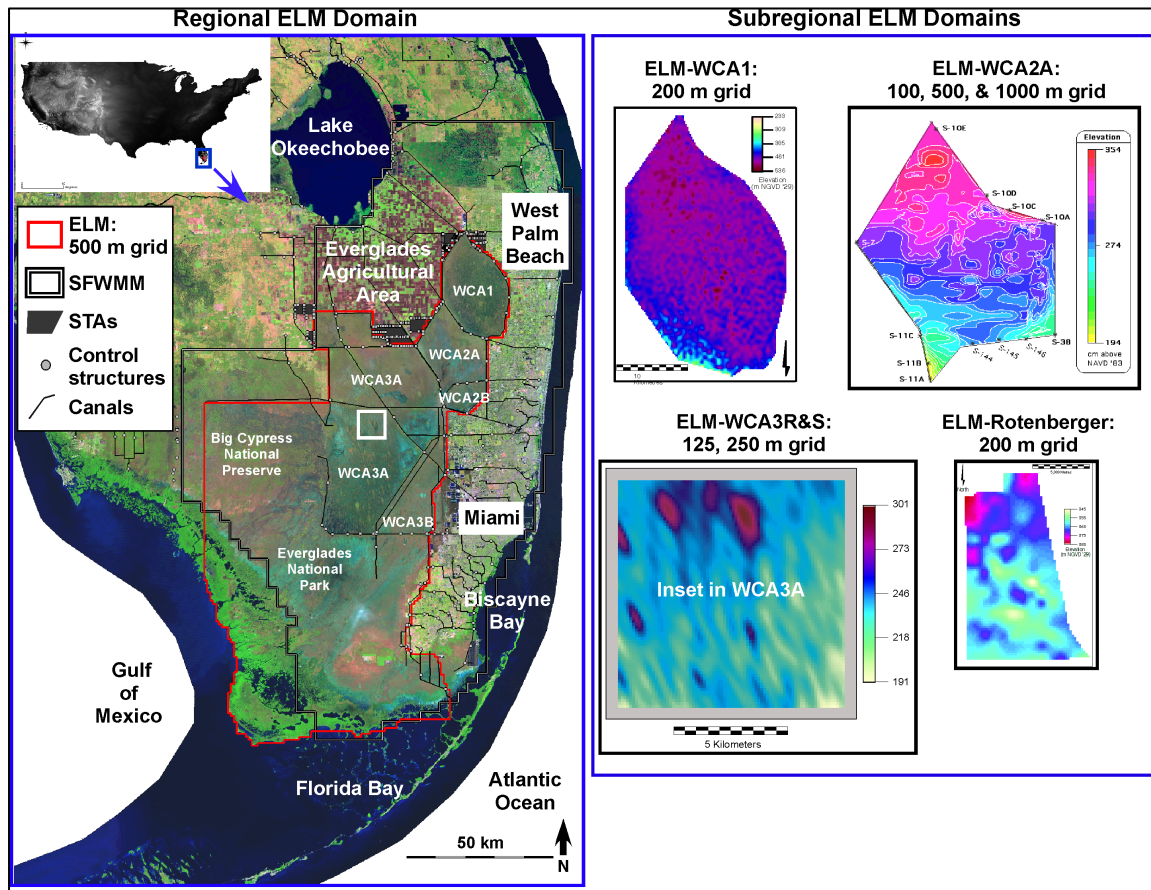
All spatial data are referenced to zone 17 of the Universal Transverse Mercator (UTM) geographic coordinate system, relative to the 1927 North American Datum (NAD).

4.3.1.1 Regional domain (*infile = "ModArea"*)

The focus of this review is on the regional application of ELM to the greater Everglades region, from the northern Everglades marshes along the Everglades Agricultural Area to the mangroves along Florida Bay and the Gulf of Mexico. This region is generally restricted to the "natural" areas of the greater Everglades, including all of the Water Conservation Areas, Holey Land, Rotenberger Tract, most of Everglades National Park, and most of Big Cypress National Preserve (Figure 4.1). This regional application uses 0.25 km² square grid cells that encompass an area of 10,394 km² (4,013 mi²). The 1 km regional application uses the same domain extent, but with 1 km grid resolution. All of the maps of the regional application are bounded by the following rectangle of UTM coordinates in zone 17 (NAD 1927):

northing:	2,952,489 m
southing:	2,914,489 m
easting:	578,711 m
westing:	553,711 m

Figure 4.1. The regional and subregional domains of the ELM, and the regional domain of the South Florida Water Management Model (SFWMM).

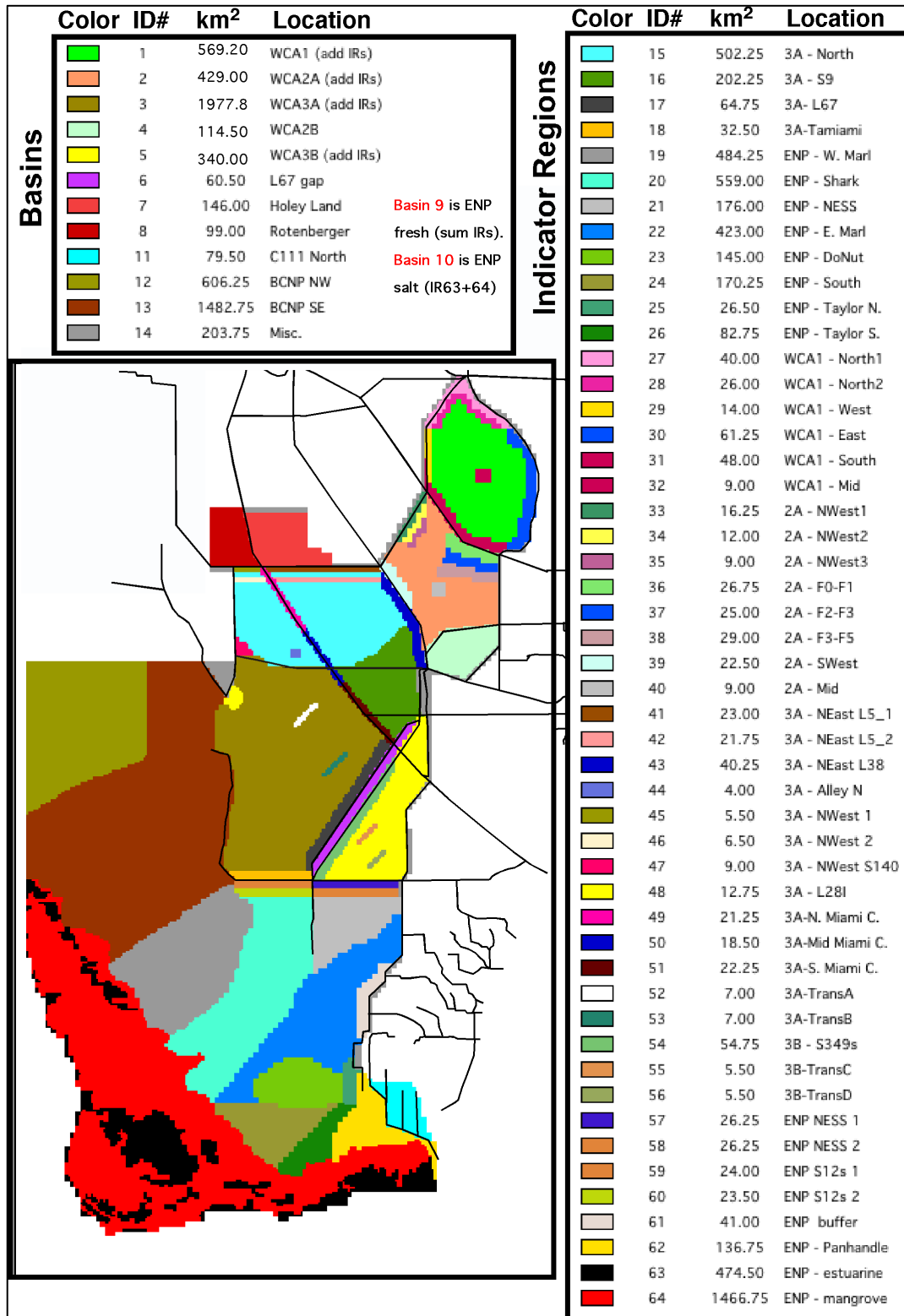


4.3.1.2 Basins & Indicator Regions (*input = "basins", "basinIR"*)

The map of the 64 Basins and Indicator Regions defines the spatial distribution of hydrologic Basins and Indicator Regions (BIR). **These BIR spatial distinctions do not affect any model dynamics**, but are used in summarizing constituent & water budgets and selected ecological Performance Measures. Budgets and Performance Measure variables are output at the different spatial scales defined by the BIR. The Indicator Regions are particularly useful for summarizing model dynamics along hydro-ecological gradients.

The largest spatial unit is Basin 0, the "basin" of the entire domain. Hydrologic basin(s) within the domain are regions with either complete restrictions on overland flows (such as Water Conservation Area 1 surrounded by levees) or partial restrictions of overland flows (i.e., Water Conservation Area 3A is bounded by levees except along part of its western boundary). Hydrologic basins are "parent" regions that (may) contain "child" Indicator Regions. Indicator Regions are drawn within a hydrologic basin boundary (but an Indicator Region may not belong to two parent basins). In reporting BIR output data, parent basins' data include (e.g., sum) the data on all child Indicator Regions contained within them. The Indicator Regions may be defined in any configuration desired for a project's objectives.

Figure 4.2. An example of a Basin and Indicator Region (BIR) map. Note that parent hydrologic Basins 1, 2, 3, 5 include multiple colored Indicator Regions, thus Basin colors show incomplete area for those Basins (but listed km² area are for total Basin). BIR map does not affect results of model calculations, and is only relevant for post-processing.



4.3.2 Temporal domain

The ELM can be applied at a variety of time scales, depending on the objective and the availability of boundary condition data. The temporal extent of the historical period used in evaluating model performance (calibration/validation) is 1981 – 2000.

The temporal extent of the available meteorological record (used in future alternative model evaluations) is 1965 – 2000. As detailed later in this Chapter for each boundary condition data file, the temporal grain of these input data is 1-day. As described in the Model Structure chapter, the time step (dt) of the vertical solutions is 1-day, while the time step for horizontal solutions varies with the model grid resolution.

While the 1-km resolution applications of ELM utilize 12 horizontal time slices per day (2-hr dt), the 500-m resolution applications utilize 40 horizontal time slices per day (36-min dt).

4.4 Initial condition maps

See *ELM v2.5 Data* and *ELM v2.8.4 Data Chapters*.

4.5 Static attributes

4.5.1 Water management infrastructure

See *ELM v2.5 Data* and *ELM v2.8.4 Data Chapters*.

4.5.2 Model parameters

As we describe below, for ELM v2.8.6 we added 1) a sulfate calibration parameter, 2) a sulfate atmospheric deposition parameter (with map option), and 3) a sulfate settling rate map.

4.5.2.1 Global parameters (input = “GlobalParms_NOM”)

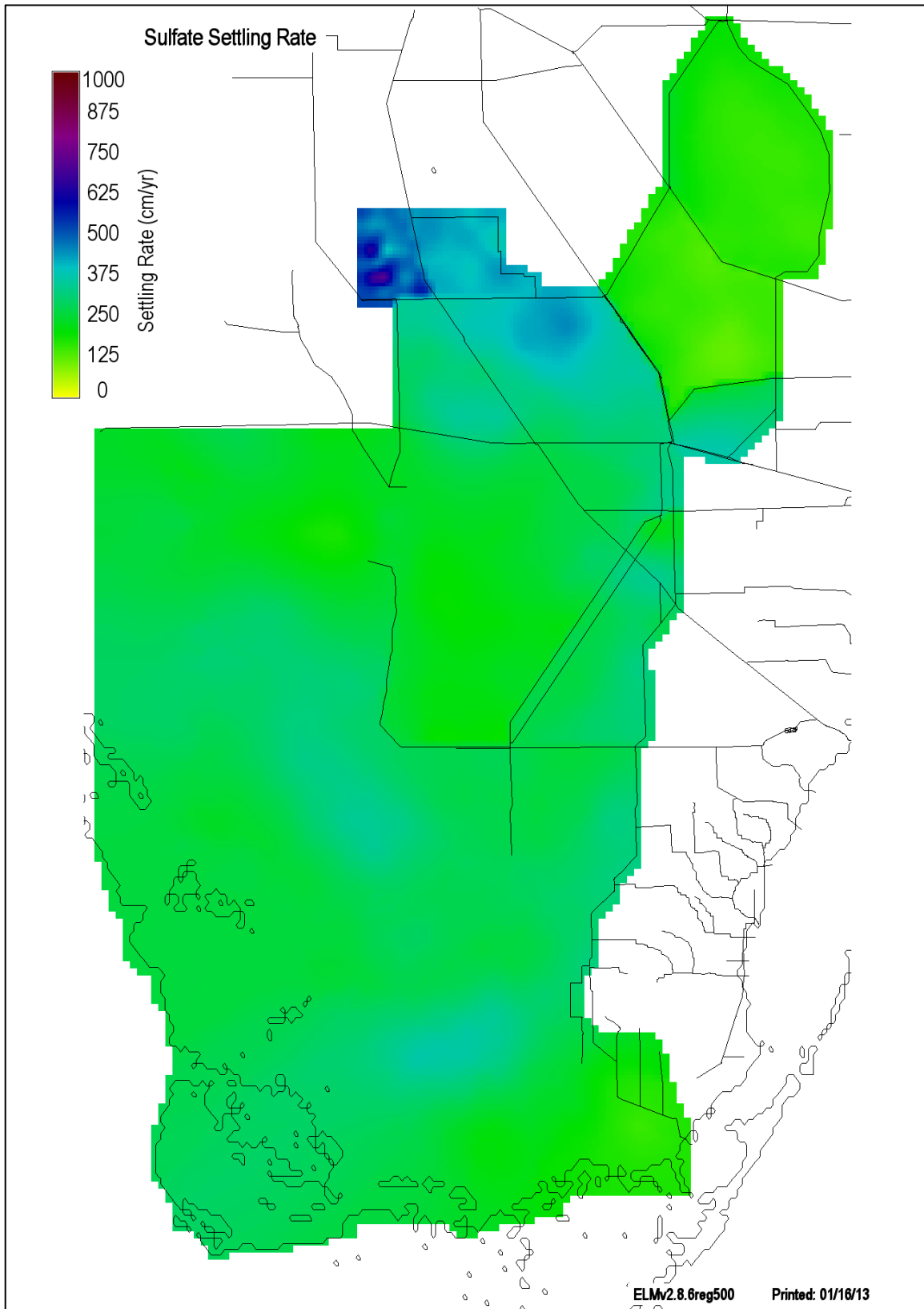
Two new global parameters were added:

- **added** "GP_SO4setMult" = 1.0 (dimless). Description: calibration multiplier of SO4 net settling rate
- **added** " GP_SO4_IN_RAIN" = 1.0 mg/L. Description: Sulfate concentration in rainfall (negative value results in code using temporally constant deposition from input map)

4.5.2.2 Sulfate settling rate map (input = “soil_SO4SetVel”)

The net settling rate for sulfate loss from the surface water (via microbial sulfate reduction in the soil) was assumed to vary in relationship to the percentage of organic matter and bulk density of the soil. The spatial map of this rate parameter was a simple multiplier of the initial soil organic bulk density (soil_orgBD in Table 1; see ELM v2.8.4 Data Chapter). The resulting settling rate varied between 114 to 717 cm/yr throughout the regional domain (Figure 4.3).

Figure 4.3. Map of the net settling rate of SO₄ loss from the surface water, used as the rate parameter for the sulfate module's net settling loss equation.



4.6 *Boundary conditions*

4.6.1 Meteorological

See *ELM v2.5 Data* and *ELM v2.8.4 Data Chapters*.

4.6.2 Hydrologic

See *ELM v2.5 Data* and *ELM v2.8.4 Data Chapters*.

4.6.3 Nutrient/constituent inflows

4.6.3.1 *Atmospheric phosphorus, chloride, and sulfate deposition*

For phosphorus and chloride, there were no change from ELM v2.8.4.

For ELM v2.8.6, we added sulfate inputs to the model from atmospheric deposition, using a rainfall concentration that was constant in time, at 1.7 mg l^{-1} (see above Model parameters section).

4.6.3.2 *Phosphorus & chloride in structure inflows (input = “CanalData.struct_TP”, “CanalData.struct_TS”)*

See *ELM v2.5 Data* and *ELM v2.8.4 Data Chapters*.

4.6.3.3 *Sulfate (SO₄) in structure inflows (input = “CanalData.struct_SO”)*

Using interpolation methods to fill in missing temporal data (see ELM v2.5 Data Chapter), we developed daily sulfate concentration time series for all water control structures that introduced "new" water into the ELM domain. These continuous daily concentration data were calculated using Microsoft Excel interpolation routines. As described for ELM v2.5, for any water control structure that had missing data at either the beginning or the end of the observed data time series, we applied the period-of-record median value.

All sulfate concentration data were acquired from the SFWMD DBHYDRO database. The period-of-record summaries for all inflow water control structures are shown in Table 4.2. **Note from that summary that the observed data are generally available on a much less frequent basis than those of total phosphorus** or chloride, and have almost an order of magnitude lower number of observations for many of the major inflow structures (relative to those for phosphorus; see ELM v2.5 Data Chapter).

Table 4.2. Summary of available observed sulfate concentration data at boundary-condition inflow water control structures, 1981-2000. N(obs) is the total number of observed sulfate samples during the 7,305-day period of record. Mean is the mean observed sulfate concentration (mg l^{-1}).

Structure	N (obs)	Mean
ACME12	15	23.5
G251	210	47.2
G200	77	33.8
G310	12	48.0
L28WQ	57	10.0
G155/L3BRS	46	10.5
S140	67	7.6
S150	55	42.1
S175	4	5.8
S18C	13	13.5
S332	9	6.5
S332D	2	4.2
S5A	97	70.1
S6	69	54.3
S7	68	51.0
S8	77	33.8
S9	62	6.8

4.7 Performance assessment targets

4.7.1 Hydrologic

See *ELM v2.5 Data* and *ELM v2.8.4 Data Chapters*.

4.7.2 Water quality

4.7.2.1 Surface water quality constituents (*added sulfate data*)

For phosphorus and chloride, there were no change from ELM v2.8.4.

For sulfate, we acquired all available observed sulfate concentration data for the marsh and canal water quality monitoring stations that were used in ELM v2.5 - v2.8.4 (see ELM v2.5 Data Chapter). Those sulfate observations were obtained from the SFWMD DBHYDRO database, along with the addition of sulfate observations from transects in WCA-1 and WCA-2A that were provided by S. Newman (SFWMD, personal communication). Basic summary statistics for those observed data may be found in the Model Performance Chapter 6, in the statistical performance table.

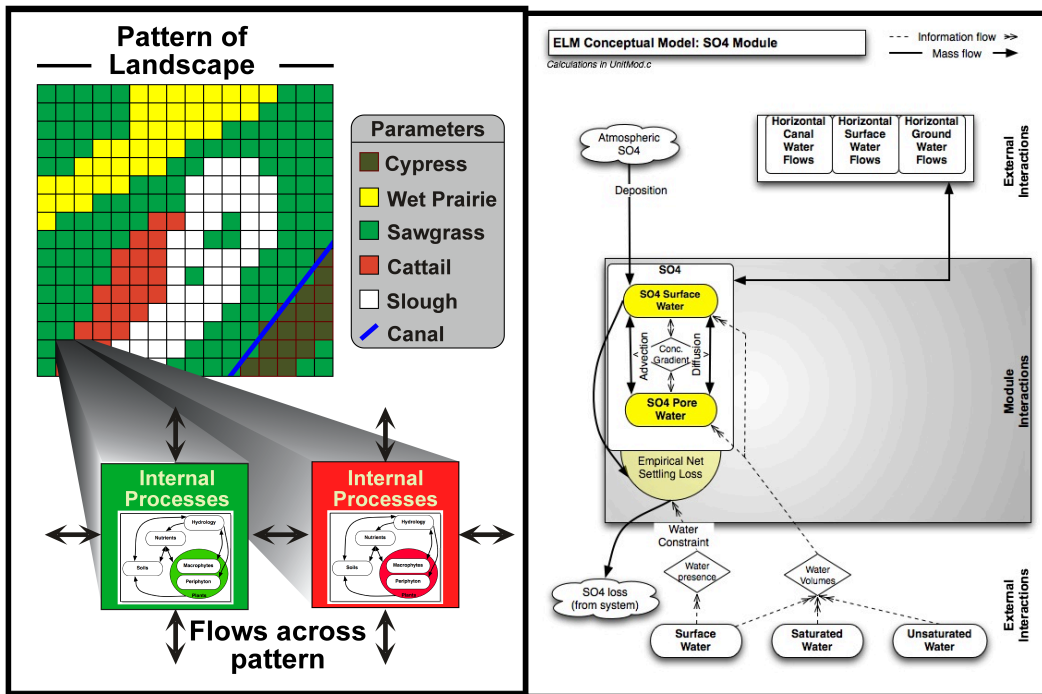
4.7.3 Ecological

See *ELM v2.5 Data* and *ELM v2.8.4 Data Chapters*.

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Documentation of the Everglades Landscape Model: ELM v2.8.6

Chapter 5: Model Structure



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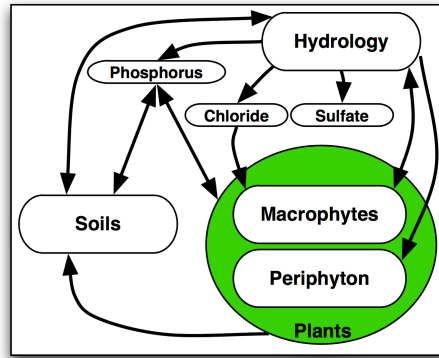
April 18, 2013

Chapter 5: Model Structure

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5.1 Overview

The focus of this Chapter is the description of a new sulfate loss module. For this ELM v2.8.6 regional application, we added a new module of sulfate losses from the surface water, and that module has no affect on any of the other simulated hydrologic, biogeochemical, or biological dynamics.



The sulfate (SO_4) module simulates the "vertical solutions" of sulfate dynamics in surface water and groundwater (saturated and unsaturated) storages within a unit grid cell. The module uses the same equations as the ELM v2.8.4 phosphorus and chloride (vertical solution) modules for a) advection of sulfate with downflows and upflows among surface and ground- water storages, and b) bi-directional diffusion of the constituent across the surface water and groundwater interface. To simulate loss of sulfate from the surface water storage due to soil microbial sulfate reduction, we assume a first-order net settling loss, aggregating all biological and biogeochemical processes in a single parameter. The sulfate loss occurs whenever surface water depth is greater than a threshold parameter value (currently 1 cm depth).

The horizontal (grid cell-to-cell) fluxes of advection and dispersion are simulated using the same equations as those for chloride and phosphorus constituents. A detailed mass-balance budget module provides the same budget (post-processing) analyses as that for chloride.

The Everglades Landscape Model (ELM) is a spatially distributed simulation using integrated hydro-ecological process modules. With a structured programming approach, the hydrologic, biogeochemical, and biological processes (such as evapotranspiration, soil oxidation, and plant growth) are contained in code modules that are activated by the user at runtime. Being "data-driven", the model relies on databases to modify scenarios of water management, while computer source code remains constant.

This Chapter on Model Structure for ELM v2.8.6 serves to update the Model Structure Chapter 5 of the ELM v2.8.4 and ELM v2.5 Documentation Reports, which are available at: <http://ecolandmod.ifas.ufl.edu/publications>. Therefore, this is not a "stand-alone" document on the overall model structure, but simply describes the new sulfate loss algorithm. For reader convenience, we also provide an updated table summarizing all code revisions since ELM v2.5.2.

5.2 Background

5.2.1 Application summary

The U.S. Army Corps of Engineers provided the funding to develop a new ELM module to simulate sulfate (SO_4) loss from the surface water. The only model structure (source code) changes for this new ELM v2.8.6 application involved those associated with the sulfate module. All of the other code (and data) used in this application remain the same as those used in the regional ELM v2.8.4, and thus documentation of those are found in prior publications: ELM v2.8.4 Documentation Report¹ and the ELM v2.5 Documentation Report².

We will apply this fine-scaled regional v2.8.6 application to help evaluate sulfate water quality responses to future management alternatives for the Comprehensive Everglades Restoration Plan (CERP) Aquifer Storage and Recovery (ASR) project. The results of that application will be posted on the EcoLandMod web site.

¹ Fitz, H.C., and R. Paudel. 2012. Documentation of the Everglades Landscape Model: ELM v2.8.4. Ft. Lauderdale Research and Education Center, University of Florida. <http://ecolandmod.ifas.ufl.edu/publications/>. 364 pp.

² Fitz, H.C., and B. Trimble. 2006. Documentation of the Everglades Landscape Model: ELM v2.5. South Florida Water Management District, <http://ecolandmod.ifas.ufl.edu/publications> (Reviewed by independent expert panel, review report at <http://ecolandmod.ifas.ufl.edu/publications>) 664 pages.

5.3 Update summary, ELM v2.5 – v2.8.6

This Model Structure Chapter 5 for ELM v2.8.6 describes ONLY changes that were made for the new sulfate module.

As summarized in Table 5.1, a variety of other modifications were made to the ELM between v2.5 and v2.8.6, the latter being the version applied for the CERP Aquifer Storage and Recovery (ASR) project.

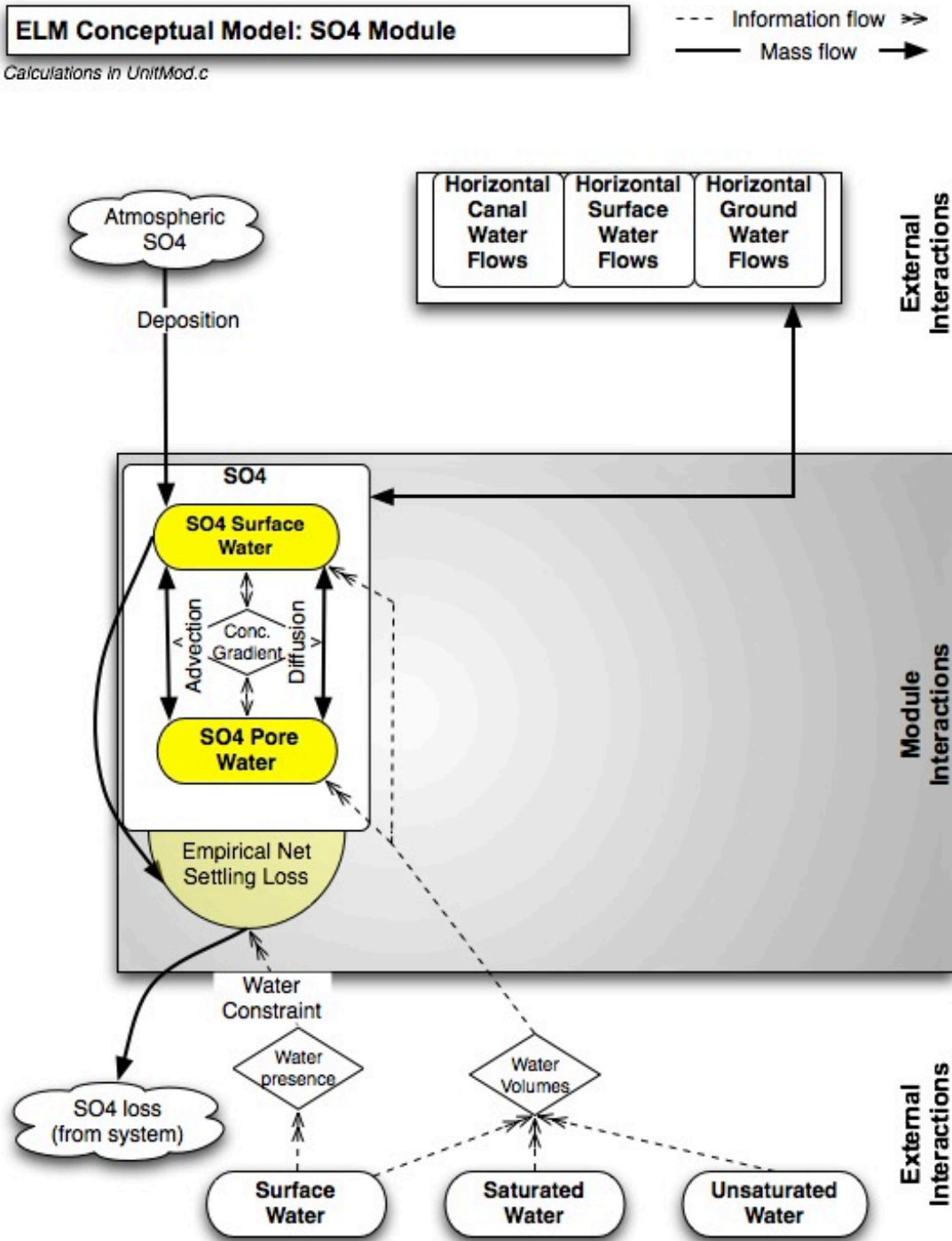
Table 5.1. Summary of updates to code for ELM applications, v2.5 through 2.8.

Version	Date	Purpose	Description/detail
2.5.2	Jul-06	Public release	Complete documentation, source code, data for regional application
2.6.0	Nov-06	Expand functionality	In response to Peer Review Panel requests, modified input/output utility functions, for greater flexibility in boundary conditions <i>a) new data for Ridge&Slough subregional application, century time scales</i>
2.6.1	Jan-07	Documentation update	Following Peer Review project, misc updates to code and data documentation, for finalizing results of Peer Review project
2.7.a	Jul-07	No code changes	New spatial data, for prototype of new regional application at 500 m grid resolution; improved model-installation methods
2.7.0	Oct-07	Expand functionality; bug fixes	Formalize velocity calculations for sediment transport; enhance multi-grid modeling capabilities <i>a) increased number of point time series locations that may be output;</i> <i>b) corrected stage vs. depth code for overland flows from SFWMM at domain periphery (identified during Peer Review)</i> <i>c) corrected code that was intended to “auto-scale” constituent dispersion at different grid resolutions (identified during Peer Review)</i> <i>d) option to output surface water flow velocities in grid cells</i>
2.7.1	Nov-07	Expand functionality	Prototyping for increased flexibility in water management options (designing to be limited in scope/complexity) <i>a) prototype restructuring of modules for rule-based water control structure flow</i> <i>b) option to output grid-cell information from boundary-condition model (e.g., SFWMM)</i>

Table 5.1 (continued). Summary of updates to code for ELM applications, v2.5 through 2.8.

Version	Date	Purpose	Description/detail
2.8.0	Dec-07	No code changes	New land surface elevation map & new vertical datum, for optional use in new regional application at 500 m grid resolution
2.8.1	Feb-08	Expand functionality	Completed update to rule-based water management modules; other extensions to capabilities <i>a) increased modularity to support expanded capabilities in triggering rule-based managed flows</i> <i>b) added chloride atmospheric deposition equation and supporting dbase change</i> <i>c) added option to output new Basin/Indicator-Region file; extended option to output boundary-condition model data (e.g., NSM/SFWMM)</i>
2.8.2	Jul-08	Expand functionality	Additional spatial array (map) output capabilities <i>a) added floating point spatial array output options</i> <i>b) added self-documenting netCDF spatial array output options</i> <i>c) added units to Model.outList (runtime configuration) file, to support self-documenting netCDF format</i>
2.8.3	Feb-09	Public release	Documentation for public release, regional and subregional applications
2.8.4	Jan-12	Public release	Documentation for public release, regional and subregional applications. ELM v2.8.4 is used in CERP Decomp project (Minor changes to some data, added model performance analysis, changes to user-guide. Minor version documentation update provided for complete documentation of version used in CERP Decomp)
v2.8.6	Jan-13	Expand functionality	Documentation for new sulfate water quality module, regional (and subregional) applications. ELM v2.8.6 is used in CERP ASR project. (Minor version documentation updated provided for complete documentation of version used in CERP ASR)

5.4 Sulfate loss module (v2.8.6)



5.4.1 Overview: Sulfate Module

This Module serves to update the constituent state variables of sulfate, in vertical fluxes among the surface water and groundwater sulfate storages and external sources/sinks of sulfate. Microbial sulfate reduction (loss, to sulfide) occurs in anoxic soils/sediments, which is associated with flooded wetlands. Sulfate reduction is of interest relative to a variety of marsh biogeochemical processes, in particular because sulfate-reducing bacteria produce methylmercury (MeHg) that can be bioaccumulated in marsh-resident animals. Anthropogenic (manmade) loading of sulfate stimulates MeHg production, as management of flows through water control structures and canals (Water Management Modules) has significantly modified the distribution of sulfate loads and concentrations across the Everglades landscape.

The sulfate (SO_4) module simulates the "vertical solutions" of sulfate dynamics in surface water and groundwater (saturated and unsaturated) storages within a unit grid cell. Vertical advective and diffusive exchanges among those storages are driven by water flows and sulfate concentrations. To simulate loss of sulfate from the surface water storage due to soil microbial sulfate reduction, we assume a first-order net settling loss, assuming that all biological and biogeochemical processes are aggregated in a single net loss parameter.

Outside of the vertical solution Sulfate Module, the horizontal (grid cell-to-cell) fluxes of sulfate advection and dispersion are simulated using the same equations as those for chloride (and phosphorus) constituents. Likewise, the same methods for chloride (and phosphorus) constituent fluxes are used for the horizontal canal (and canal-cell) sulfate fluxes.

A detailed mass-balance budget module provides the same budget (post-processing) analyses as those for chloride.

5.4.2 Sulfate Module description

As a part of the broader objective of capturing inter-annual and seasonal trends in the regional gradients of this constituent, the principal objective of the Sulfate Module is to simulate a) vertical atmospheric deposition, b) the vertical diffusive and advective fluxes, and c) net loss of sulfate from the system via a first-order net settling rate approach.

Total atmospheric deposition of sulfate is considered by applying a constant concentration to rainfall that results in a long term, domain-wide annual deposition rate of approximately $1.3 \text{ g SO}_4/\text{m}^2/\text{yr}$ in the current model version (using 1.0 mg/L rainfall SO_4 concentration, Data Chapter 4).

This module considers the downward advection of constituents from surface water storage, and the bi-directional diffusive flux across the ground (soil/sediment) and surface water storages. Upflow due to horizontal subsurface flows are accommodated in the integration of surface water and groundwater in the Groundwater Flux Module.

To simulate loss of sulfate from the surface water storage due to soil microbial sulfate reduction, we assume a first-order net settling loss, aggregating all biological and biogeochemical processes in a single parameter, which is a spatially distributed map parameter that ranges between approximately 1 to 7 m/yr across the region (see Data

Chapter 4). The sulfate loss occurs whenever surface water depth is greater than a threshold parameter value (currently 1 cm depth, see Data Chapter 4).

5.4.3 Sulfate Module Equations

All vertical solution modules are processed within a spatial loop across columns and rows of the model grid (see ELM v2.5.2 Documentation Report, Chapter 5 Model Structure). For each grid cell address (`cellLoc`), whenever the surface water depth exceeds the threshold depth (`GP_WQualMonitZ` (m), a Global Parameter in `GlobalParms_NOM`, see Data Chapter 4), the potential sulfate loss (`SO4_settl_pot`, kg/d) from the surface water storage is calculated by:

$$1) \text{SO4_settl_pot} = \text{SO4settlVel}[\text{cellLoc}] * \text{CELL_SIZE} * \text{SO4_SF_WT_mb}[\text{cellLoc}]$$

where

`SO4settlVel`[`cellLoc`] is the net settling rate (m/d) parameter at grid cell address `cellLoc` (from input map `soil_SO4SetVel`, see Data Chapter 4),

`CELL_SIZE` is the surface area of a grid cell (m^2), and

`SO4_SF_WT_mb`[`cellLoc`] is the sulfate concentration (kg/m^3) in surface water at grid cell address `cellLoc`, previously calculated from the current water volume and sulfate mass in the grid cell.

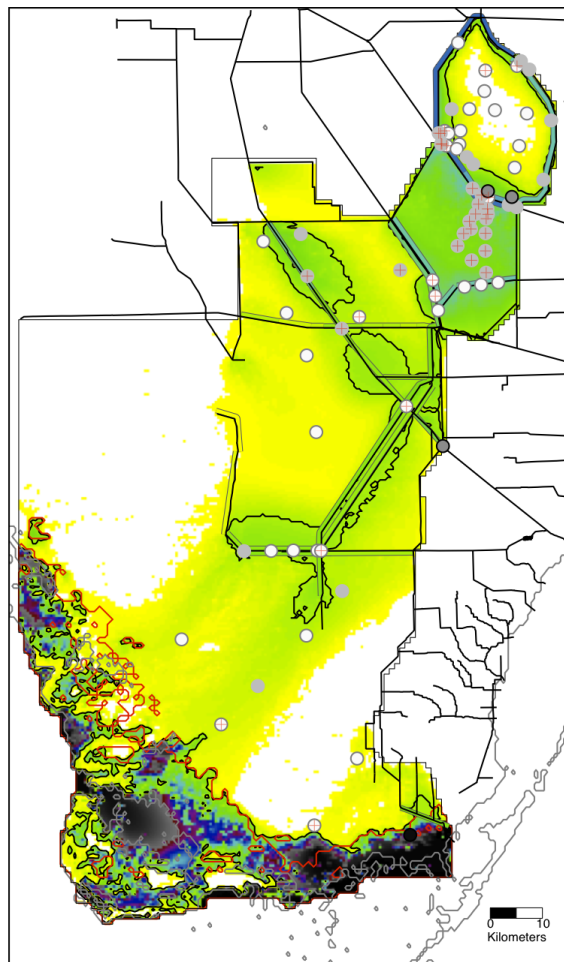
The state variable of sulfate mass storage in the grid cell, `SO4_SURF_WT`[`cellLoc`], is then updated in the state variable's difference equation, with a mass balance constraint that the potential loss of `SO4_settl_pot` (kg/d) cannot exceed the current mass of `SO4_SURF_WT`[`cellLoc`] (kg).

Other equations associated with atmospheric deposition and vertical advection and diffusion are the same form as those used in the Phosphorus Module and Salt/Tracer Module (see ELM v2.5.2 Documentation Report, Chapter 5 Model Structure).

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Documentation of the Everglades Landscape Model: ELM v2.8.6

Chapter 6: Model Performance



<http://ecolandmod.ifas.ufl.edu>

April 18, 2013

Chapter 6: Model Performance

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6.1 Overview

As described in the Introduction Chapter 1 of the ELM v2.5 Documentation, an overarching goal of the ELM is to understand and predict ecological dynamics across the greater Everglades landscape. For the current ELM v2.8.6, we added a new module for marsh sulfate dynamics, expanding on the functionality of the ELM.

In its regional (~10,000 km²) application at 0.25 km² grid resolution, the current ELM version 2.8.6 was developed to assess relative differences in sulfate dynamics associated with Everglades water management plans - at decadal time scales. As described in the Model Structure Chapter 6, the sulfate module does not affect any other hydro-ecological modules in the ELM (documented in the last update, ELM v2.8.4). In this update to ELM v2.8.6, we maintained all data that affected the previously-documented calibration/validation hydro-ecological performance characteristics of the model. Therefore, this model performance update applies only to the newly added sulfate module.

The overall approach of (developing and) calibrating the ELM for hydro-ecological dynamics was described in Chapter 6 of the ELM v2.5 Documentation Report. For this update, we developed and calibrated the new sulfate module, using the same graphical and statistical methods used previously for other water quality (phosphorus and chloride) constituents.

The sulfate model performance characteristics (with moderate rates of microbially-mediated losses) were expected to be similar to those of the conservative tracer of chloride, and the rapidly-assimilated phosphorus marsh dynamics (due to high uptake and cycling via microbial and plant utilization).

The sulfate module met those performance expectations. The **median seasonal relative bias (observed minus simulated) of sulfate predictions for all stations was 0 mg L⁻¹ in marshes and -2 mg L⁻¹ in canals**; the median seasonal relative bias was -12% and -8% in the marsh and canals, respectively. For comparison, the median seasonal relative bias in chloride predictions was 11% in both the marsh and canals, with the same phosphorus prediction statistics being 1% and 2% in marshes and canals, respectively.

Thus, the model “skill” in predicting landscape sulfate dynamics at these decadal time scales is consistent with other model performance characteristics. Given these successful performance results, we are using this fine-scaled regional application to help evaluate landscape sulfate water quality responses to future management alternatives for the Comprehensive Everglades Restoration Plan (CERP) Aquifer Storage and Recovery (ASR) project.

NOTE on this Model Performance Chapter 6 update: the following sections are mostly copies of text from ELM v2.5.2 and v2.8.4 documentation, and are provided simply for reader convenience: Sections 6.2 (Performance expectations), 6.3 (Performance evaluation methods), 6.4 (Model updates), and 6.5 (Model configuration)

6.2 Performance expectations

6.2.1 Model application niches

For model users and stakeholders, a fundamental concern is simply: how well does the model work? To be useful, it is critical that model goals and objectives are clearly stated, and that the design and performance of the model is shown to meet those goals.

Towards this end, it is critical that a model is understood within the context of its “application niche”. The application niche should be a juxtaposition of A) the real or perceived needs of the “users” and B) the realistic capabilities portrayed by the model developers. The intersection of A & B is the intended target of the model application – a basic point that is sometimes lost in practice as a result of inadequate communication.

6.2.2 ELM v2.8 application niche

The ELM application niche is broadly defined as that which improves our understanding of hydro-ecological dynamics, with the current ELM v2.8.6 emphasis on those that relate to water quality - specifically sulfate. The model Performance Measures to be used in comparing relative benefits of alternative management plans define the specific Objectives of the model, including the spatio-temporal scale of application. While the ELM is designed to address a larger suite of ecological questions, the relatively narrower subset of *current* model Objectives should be considered to be the *current* application niche of the ELM.

An overarching Goal of the ELM is to understand and predict ecological dynamics across the greater Everglades landscape. For the current ELM v2.8.6, we emphasize that the available ecological Performance Measures are those involving the “water quality” aspect of ecosystem dynamics across the landscape, with an **emphasis on sulfate dynamics**.

6.2.3 Establishing performance expectations

6.2.3.1 ELM

The expectations of hydrologic simulations in the Everglades are reasonably well-understood by most users. Perhaps this is largely due to the context of hydrologic modeling in south Florida, which has a multi-decadal history of applications, with a relatively well monitored system in which the physics are reasonably well understood.

There is less of a common understanding of the expected performance of regional Everglades models that simulate ecological (including water quality) dynamics. Nutrients are subject to many more processes (such as uptake by plants, release by soils, etc.) than are water depths. Moreover, there is about an order of magnitude fewer observed data available relative to hydrologic data (in the Everglades): the quantity of water flowing into a basin may be reasonably well-known on a daily basis, but the associated nutrients (and other water quality constituents of chloride and sulfate) are generally sampled less than 5 - 10% of that time (see the Data and the Uncertainty Chapters of ELM v2.5 documentation). Observations in the marsh, used to compare to the model output, can be even less frequent than those input data.

This combination of very infrequent data collections in the Everglades, along with highly-variable, random processes, leads to relatively high uncertainties in analysis

of water quality performance, and necessitates the more complex assumptions for any water quality or ecological model relative to those involving physical hydrology.

6.3 Performance evaluation methods

The methods of evaluating and improving the performance of a distributed, integrated ecological model are wide ranging, usually involving both analytic tools and science-based judgments. Ultimately one seeks to communicate the cumulative evidence of how well the model meets its objectives: an evaluation of the model performance in history-matching is a fundamental component of that communication.

Because we **have not attempted to "re-calibrate"** the (non-sulfate) hydro-ecological dynamics of ELM as data and code were updated from v2.5 to v2.8, please see **Chapter 6 of the ELM v2.5 Documentation Report for the discussion of the calibration process, validation process, and performance evaluation methods** (pp. 6-5 through 6-14). The statistical metrics used in evaluating model performance are repeated in this ELM v2.8.6 chapter as Appendix A.

6.4 Model updates

As described in other Chapters, the current release¹ ELM v2.8 has a number of improvements over the last release, ELM v2.5. For the source code (Chapter 5), several changes were made to accommodate specific objectives of evaluating local scale management alternatives. As described in that chapter, the principal changes were made to increase the functionality of the model in simulating managed flows through water control structures. In maintaining its design goals, the ELM v2.8 code remains general in scope, such that a change made to accommodate such new functionality does not affect other applications if that functionality is not needed. Thus, when referring to v2.8 of the ELM code, it does not matter whether the model project of interest is a regional or subregional application – the algorithms and code are general to all.

The new fine resolution regional model (ELM v2.8) encompasses a domain identical to the regional ELM v2.5 (10,394 km²), but with 42,576, 0.25 km², active grid cells (four times the 10,394 grid cells in the 1 km² resolution version). For this ELM v2.8 regional application, most of the data (Chapter 4) remain the same as those used for the ELM v2.5 regional application. The principal changes involved “resampling” data from the 1 km resolution map inputs, and generating new spatial interpolations of the updated land surface elevation data at the 500 m resolution.

For the update from ELM v2.8.4 to v2.8.6, we added the new sulfate module (see Model Structure Chapter 5, and Data Chapter 4).

6.5 Model configuration

In ELM v2.8, the model was configured to simulate historical conditions inclusive of the years 1981 – 2000. The domain was that of the regional ELM, employing a 0.25 km²

¹ For simplicity, any full public release version is denoted only by the primary and secondary version attributes (see Model Refinement Chapter, ELM v2.5 Documentation). The tertiary version attribute of this model release is ELM v2.8.6.

grid mesh encompassing all of the Water Conservation Areas, Holey Land, Rotenberger Tract, parts of the Model Lands near the C-111 canal region, and most of Everglades National Park and Big Cypress National Preserve. The vector topology of the canal/levee network and the point locations of water control structures were constant during the simulation period. The habitat succession module was operating, as were all other ecological (including sulfate) modules, providing dynamic feedbacks among the physics, chemistry, and biology of the mosaic of ecosystems in the landscape.

However, the new **sulfate module does not affect any other module in ELM.**

Dynamic boundary conditions included daily data on rainfall, potential evapotranspiration, managed water control structure flows with associated constituent concentrations, and stage (along the borders of the domain, including annually-recurring, monthly mean tidal amplitudes). Full descriptions of the requisite data and the functionality of the algorithms and source code are provided in other Chapters of this documentation.

6.6 Performance results

6.6.1 Ecological performance

Evaluations of the full range of ecological performance measures (such as vegetation succession) were not part of the current objectives for ELM v2.8.6 application, which focused solely on sulfate water quality dynamics. Thus, here we present the performance analyses pertaining to those sulfate water quality dynamics.

6.6.1.1 Surface water sulfate (SO_4) concentrations: statistical metrics

The 78 marsh and canal water quality monitoring locations used in evaluating the model hindcasting performance (i.e., calibration) for surface water sulfate (SO_4) concentration predictions during 1981-2000 are mapped in Figure 6.4 (and 6.4b).

The seasonal relative bias metric (observed minus simulated) indicated a distribution of relative errors (Figure 6.5) that tended to be higher in close proximity to higher concentrations in canals, an expected trend that was very similar to the trends of chloride and phosphorus concentrations. The **median seasonal bias was 0 mg L⁻¹ in the marsh, and -2 mg L⁻¹ in the canals** (Table 6.1). The median seasonal relative bias of all stations was -12% in the marshes, and -8% in canals.

For comparison among sulfate, chloride and phosphorus water quality variables: the median seasonal bias in chloride predictions was 11% in both the marsh and canals, with the same phosphorus prediction statistics being 1% and 2% in marshes and canals, respectively.

The distribution of simulated sulfate concentrations throughout the freshwater Everglades showed patterns of long-term sulfate distributions (Figure 6.5) that were consistent with our understanding of major sulfate patterns related to flow distributions through the regional landscape. Examples include the localized band of high sulfate concentrations encircling WCA-1, overall high concentrations in WCA-2A, and gradients of decreasing

concentrations from the northern Everglades to downstream areas in Everglades National Park².

² The distribution of SO_4 concentrations go “off-the -scale” in the estuarine southern Everglades, with SO_4 concentrations that were $\gg 1000 \text{ mg L}^{-1}$ (1 ppt) generally corresponding to the extent of mangrove and other estuarine habitat types.

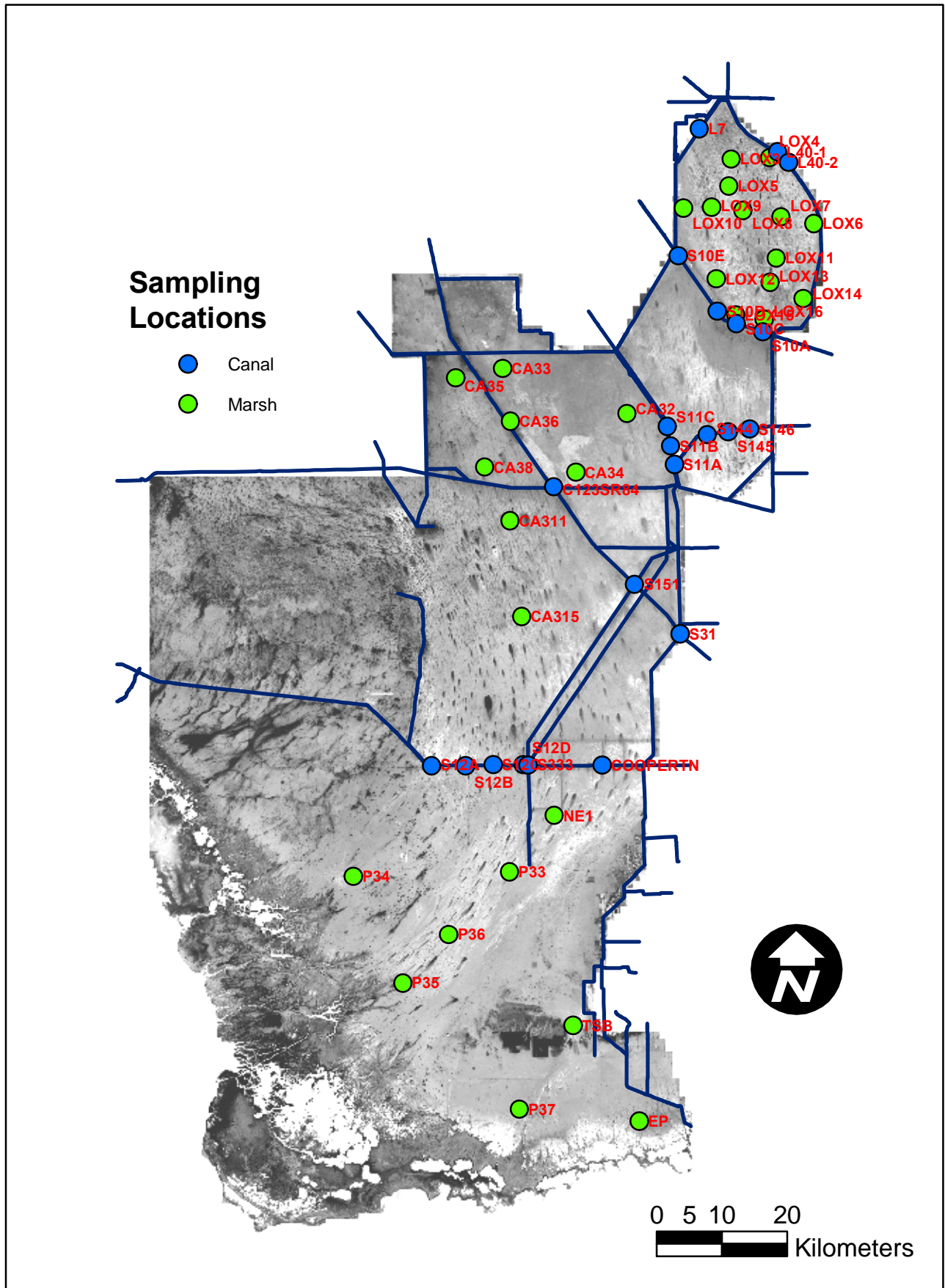


Figure 6.4 Map of most water quality monitoring site locations (see also Figure 6.4b).

Figure 6.4b. Map of water quality monitoring locations in WCA-1 and WCA-2A.

Note: the grid that is shown is 1 km², which is four times coarser than the 0.25 km² scale of the current model.

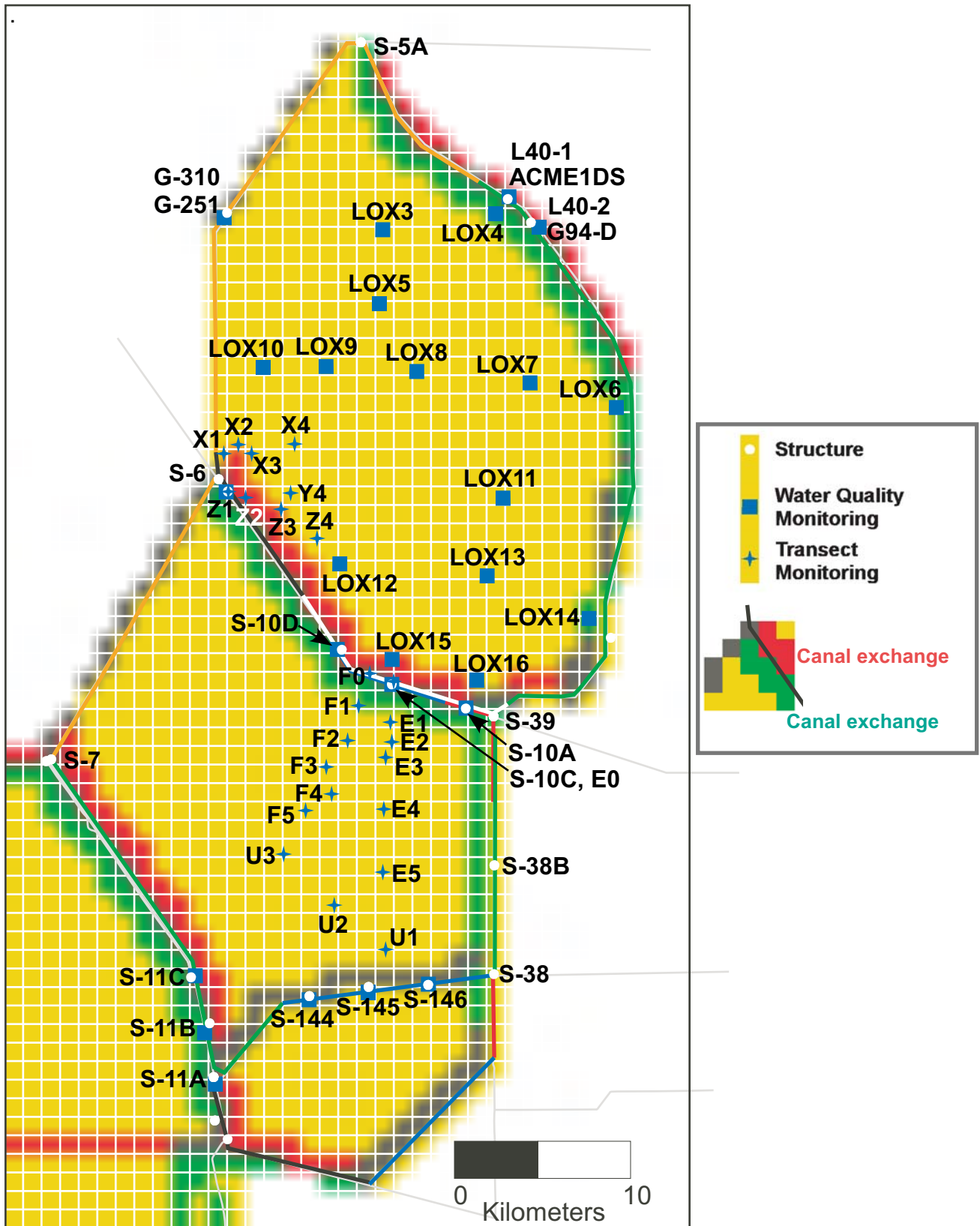


Figure 6.5 Map of seasonal bias in model predictions of observed surface water sulfate concentrations in marsh and canal locations. Background map is the simulated mean monthly SO₄ concentration during 1981-2000. Statistics are detailed in Table 6.1

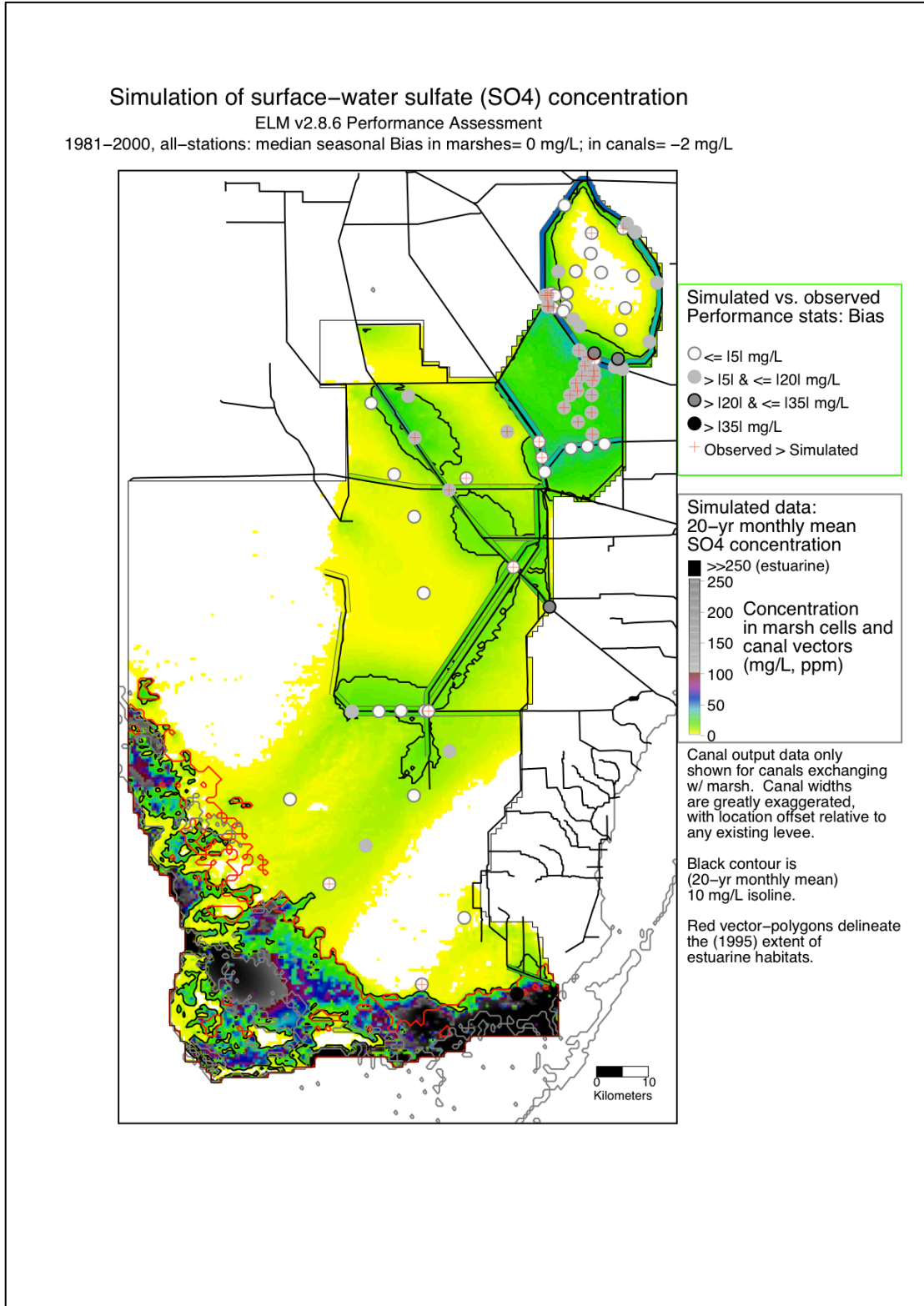


Table 6.1. Statistical evaluation of (ELM v2.8.6) simulated vs. observed seasonal surface water sulfate concentration, 1981 – 2000. Units of ObservedMean, Bias (observed minus simulated) and RMSE are mg l^{-1} (ppm); RelativeBias is proportion relative to observed mean.

Site	Basin	Site type	1981-2000				
			N	ObsMean	RelBias	Bias	RMSE
LOX4	WCA1	Marsh	11	24	0.10	2	11
LOX3	WCA1	Marsh	8	4	0.06	0	2
LOX5	WCA1	Marsh	7	1	-0.29	0	0
LOX10	WCA1	Marsh	10	11	-1.24	-14	15
LOX9	WCA1	Marsh	9	2	-1.91	-3	4
LOX8	WCA1	Marsh	10	1	-0.53	-1	1
LOX7	WCA1	Marsh	12	1	-0.88	-1	1
LOX6	WCA1	Marsh	14	6	-1.19	-7	9
X2	WCA1	Mar. Trans.	10	32	0.06	2	8
X4	WCA1	Mar. Trans.	10	7	-0.47	-3	5
X1	WCA1	Mar. Trans.	10	48	0.24	12	13
X3	WCA1	Mar. Trans.	10	23	-0.16	-4	11
Z1	WCA1	Mar. Trans.	10	48	0.34	16	18
Z2	WCA1	Mar. Trans.	10	35	0.11	4	13
Y4	WCA1	Mar. Trans.	10	8	-0.41	-3	6
LOX11	WCA1	Marsh	11	1	-0.57	-1	1
Z3	WCA1	Mar. Trans.	10	14	-0.09	-1	9
Z4	WCA1	Mar. Trans.	10	4	-1.91	-7	8
LOX12	WCA1	Marsh	14	4	-1.82	-7	8
LOX13	WCA1	Marsh	11	1	-2.48	-3	3
LOX14	WCA1	Marsh	14	3	-4.54	-12	13
LOX15	WCA1	Marsh	14	15	-1.51	-22	24
LOX16	WCA1	Marsh	13	2	-12.37	-28	28
F1	WCA2A	Mar. Trans.	12	54	0.26	14	17
E1	WCA2A	Mar. Trans.	14	47	0.12	5	12
F2	WCA2A	Mar. Trans.	14	53	0.20	11	15
E2	WCA2A	Mar. Trans.	14	48	0.16	8	14
E3	WCA2A	Mar. Trans.	14	49	0.19	9	14
F3	WCA2A	Mar. Trans.	14	54	0.31	17	19
F4	WCA2A	Mar. Trans.	14	56	0.33	19	20
CA33	WCA3A	Marsh	14	12	-0.72	-9	12
F5	WCA2A	Mar. Trans.	14	54	0.34	18	20
E4	WCA2A	Mar. Trans.	14	46	0.22	10	14
CA35	WCA3A	Marsh	12	10	-0.18	-2	9
U3	WCA2A	Mar. Trans.	14	50	0.36	18	19
E5	WCA2A	Mar. Trans.	14	45	0.26	12	15
U2	WCA2A	Mar. Trans.	14	49	0.38	19	20
CA32	WCA3A	Marsh	12	12	0.52	6	11
U1	WCA2A	Mar. Trans.	14	36	0.17	6	9
CA36	WCA3A	Marsh	12	33	0.42	14	16
CA38	WCA3A	Marsh	14	4	-0.27	-1	3
CA34	WCA3A	Marsh	13	14	0.06	1	9
CA311	WCA3A	Marsh	14	3	-0.85	-2	3
CA315	WCA3A	Marsh	14	3	-0.42	-1	3

Table 6.1 - continued. Statistical evaluation of (ELM v2.8.6) simulated vs. observed seasonal surface water sulfate concentration, 1981 – 2000. Units of ObservedMean, Bias (observed minus simulated), and RMSE are mg l^{-1} (ppm); RelativeBias is proportion relative to observed mean. *Note: the canal station "L7" had an insufficient number of observed samples to calculate these statistics. However, the overall observed and simulated means were 49 and 58 mg l^{-1} , respectively.*

NE1	ENP	Marsh	24	6	-0.92	-6	11
P33	ENP	Marsh	28	7	-0.38	-3	8
P34	ENP	Marsh	5	3	-0.83	-3	8
P36	ENP	Marsh	24	4	-1.26	-5	7
P35	ENP	Marsh	25	9	0.21	2	16
TSB	ENP	Marsh	26	6	-0.07	0	4
P37	ENP	Marsh	11	5	0.32	2	5
EP	ENP	Marsh	27	12	-5.07	-60	66
L7	WCA1	Canal	2	49			
L40-1	WCA1	Canal	7	20	-0.93	-19	20
L40-2	WCA1	Canal	7	20	-0.95	-19	21
S10A	WCA1	Canal	10	33	-0.21	-7	15
S10C	WCA1	Canal	10	42	-0.04	-2	16
S10D	WCA1	Canal	17	54	0.13	7	15
S39	WCA1	Canal	15	35	-0.20	-7	14
S10E	WCA1	Canal	7	53	0.12	6	11
X0	WCA1	Can. Trans.	10	53	0.16	9	11
Z0	WCA1	Can. Trans.	10	53	0.17	9	10
E0	WCA2A	Can. Trans.	14	49	0.07	4	11
F0	WCA2A	Can. Trans.	14	53	0.13	7	13
S144	WCA2A	Canal	12	33	-0.11	-4	12
S145	WCA2A	Canal	14	31	-0.15	-5	12
S146	WCA2A	Canal	10	31	-0.11	-3	12
S11A	WCA2A	Canal	14	33	-0.08	-3	11
S11B	WCA2A	Canal	14	38	0.07	3	13
S11C	WCA2A	Canal	17	37	0.04	2	7
C123SR84	WCA3A	Canal	10	25	0.31	8	18
S151	WCA3A	Canal	13	23	0.13	3	10
S12A	WCA3A	Canal	5	5	-1.88	-10	12
S12B	WCA3A	Canal	6	7	-0.60	-4	8
S12C	WCA3A	Canal	7	11	-0.32	-4	9
S12D	WCA3A	Canal	11	15	-0.11	-2	8
S333	WCA3A	Canal	9	16	0.12	2	8
S31	WCA3B	Canal	11	17	-1.22	-20	29
Median All:			12	20	-0.09	-1	11
Median Canal:			10	33	-0.08	-2	12
Median Marsh:			14	11	-0.12	0	11

6.6.1.2 Surface water sulfate (SO_4) concentration: graphical indicators

These visualizations of the temporal trends in simulated and observed data are an important component of understanding the model performance, particularly with respect to recognizing any unique aspects of the data dynamics at a particular site. As an example, Figure 6.6 shows the time series of seasonally-averaged sulfate concentrations in a canal compared to a downstream marsh. The model effectively captured the spatial gradient trend between the high concentrations in a WCA-2A canal (mean concentration = 37 mg L^{-1}), to a downstream location in the WCA-3A interior marsh (mean concentration = 14 mg L^{-1}).

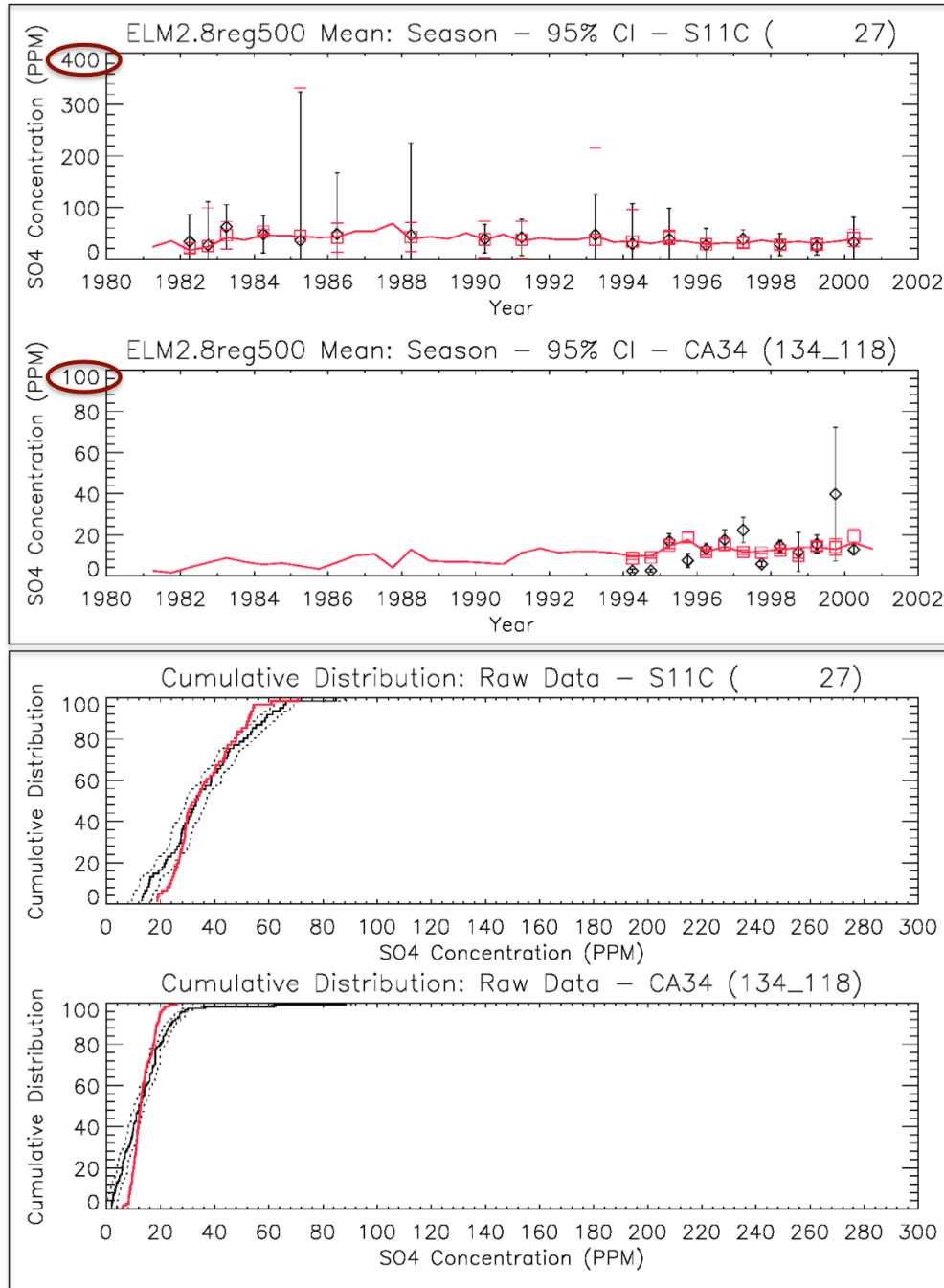
Appendix B provides all (78 sites') sets of 1981-2000 time series of observed vs. modeled surface water sulfate concentrations at varying temporal aggregations, including each site's cumulative frequency distribution.

Figure 6.6 (following page). Example plots of time series and Cumulative Frequency Distributions (CFD) of simulated and observed sulfate concentrations in canal and marsh sites.

Time series plots: All data were aggregated into arithmetic mean values by wet and dry seasons within water years; the continuous lines pass through mean of all daily data points for each season; the mean of paired **simulated** and observed values are shown in **red** boxes and black diamonds, respectively; the 95% Confidence Interval (CI) of the paired means are shown by the "___" symbols in the red for the model and black for the observed data.

Cumulative Frequency Distributions: The CFDs of the simulated and observed (raw, un-aggregated) data; the 95% confidence interval for observed data is shown in the dashed black lines. Note that only paired simulated and observed data points are used.

Figure 6.6. Time series (top) and CFDs (bottom) of simulated vs. observed sulfate concentrations for a canal site (S11C in WCA-2A, flowing into northern WCA-3A) and a downstream interior marsh site (CA34 in northern WCA-3A). Note different Y axis scales on the time series plots.



6.7 Appendix A: Computational methods for statistics

Although numerous methods exist for analyzing and summarizing model performance, there is no consensus in the modeling community on a standard analytical suite for hydrology and ecological (incl. water quality) models. It appears most useful to use a variety of methods to evaluate model performance, as no single statistic can fully capture all of the important characteristics of a comparison between the simulated and observed data. We employed the below methods to estimate Bias, RMSE, R^2 , and NS Efficiency in assessing some aspects of the model performance relative to observed data.

Bias:

$$\text{Bias} = \frac{\sum (x - y)}{n}$$

Where x is the field-observation values, y is the model-prediction values, and n is the number of observations.

Bias is calculated as the mean differences between paired modeled and observed values. It is a measure of how biased the overall values simulated by the model from the observed values. The bias should be as close to zero as possible.

Root Mean Square Error (RMSE):

$$\text{RMSE} = \sqrt{\frac{\sum (y - x)^2}{n}}$$

Where x is the field-observation values and y is the model-prediction values.

RMSE is the square root of the average values of the prediction errors squared. RMSE measures the discrepancy between modeled and observed values on an individual level to indicate accuracy of model predictions. Because of the quadratic term, RMSE gives greater weight to larger discrepancies than smaller ones. The RMSE should be as close to zero as possible.

Pearson product-moment correlation coefficient (R^2):

$$R^2 = \left(\frac{\sum (y - y_m)(x - x_m)}{\sqrt{\sum (y - y_m)^2 \sum (x - x_m)^2}} \right)^2$$

Where x_m is the observed mean of x (calculated as $\Sigma x/n$), and y_m is the model-predicted mean of observed y (calculated as $\Sigma y/n$).

The R^2 measure the degree of linear association between x and y (i.e., field observation and model predictions). It represents the amount of variability of one variable that is explained by correlating it with another variable. Depending on the strength of the linear relationships, the R^2 varies from 0.0 to 1.0, with 1.0 indicating a perfect fit.

Nash-Sutcliffe Efficiency (Eff):

$$\text{Eff} = 1 - \frac{\sum (y - x)^2}{\sum (x - x_m)^2}$$

Where x_m is the mean of the observed x , and y is the model prediction.

Like correlation coefficient, model efficiency is another overall indication of goodness of fit (Mayer and Butler 1993, Janssen and Heuberger 1995). Efficiency is equal to one minus the sum of squared prediction errors divided by the sum of squared deviation of observed values from the mean. It represents the amount of variability of one variable that is explained by modeled values. A model efficiency of 1.0 indicates a perfect fit between modeled and observed values, and a efficiency of 0.0 indicates the fit to $y = x$ is no better than $x = x_m$.

6.8 Appendix B: Time series & CFDs: SO₄

Figures B.1 – B.78. Time series plots of water column sulfate (SO₄) concentration and their associated Cumulative Frequency Distributions (CFD) for the period of record 1981-2000 at each monitoring location. The sequence of the figures is based on geographic location of marsh sites, starting in northwest, moving towards the southeast; following the set of plots of all marsh sites, the canal monitoring sites are similarly sequenced. A map of all sites is provided in the Model Performance Chapter 6.

The model grid cell column and row locations (col_row) or canal reach identifier (single integer) are shown in parentheses of each plot's title.

- a) All data were aggregated into arithmetic mean values by wet and dry seasons within water years; the continuous lines pass through mean of all daily data points for each season; the mean of paired **simulated** & observed values are shown in **red** boxes and black diamonds, respectively; the 95% Confidence Interval (CI) of the paired means are shown by the "___" symbols in the red for the model and black for the observed data.
- b) All data aggregated into arithmetic mean values by water year, with the same treatment as in plot a).
- c) The cumulative frequency distributions of the simulated and observed (raw, un-aggregated) data; the 95% confidence interval for observed data is shown in the dashed black lines. Note that only paired simulated and observed data points are used.

