Wetlands
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ORIGINAL RESEARCH

A Generalized Model of Hourly Net Ecosystem Exchange (NEE) for Florida Everglades Freshwater Wetlands

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Abstract A generalized model is presented to estimate the diurnal cycle of hourly net ecosystem exchange (NEE) based on a corresponding single reference-time observation from the Florida Everglades freshwater wetlands. The year-round diurnal cycles of NEE for two different (short vs. long hydroperiod) marsh sites were normalized by the corresponding day- and site-specific reference observations of NEE to obtain a common dimensionless cycle. An extended stochastic harmonic analysis (ESHA) was utilized to calibrate and validate the model with hourly eddy-covariance observations of NEE during 2008–13. The model involved five parameters, which exhibited spatiotemporal robustness by collapsing into narrow ranges among different days, years and sites. The daily estimates were averaged over all calibration days to calculate the site-specific ensemble parameter sets. The site-specific ensemble parameters were further averaged over four mid-day reference times (11 A.M. to 2 P.M.) across sites to obtain a generalized ensemble parameter set. Estimated hourly NEE using the site-specific and the generalized parameter sets indicated a good performance of the model (e.g., Nash-Sutcliffe Efficiency, NSE = 0.66–0.89). The model is represented in three standalone formats, including an Excel spreadsheet, to simulate the hourly NEE for the desired Julian days and years from the respective single reference observations.

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Introduction

Wetlands play an important role in the regional and global carbon dynamics due to their high rates of carbon sequestration and storage (Bridgham et al. 2006; Nahlik and Fennessy 2016). The net ecosystem exchange (NEE) of CO_2 between the vegetated wetlands and the atmosphere typically represents a concave diurnal cycle due to the daytime photosynthesis and nocturnal respiration. However, the diurnal NEE cycles of wetland ecosystems vary among different days (both intra- and inter-annually) at the same and/or different sites due to the variation in climatic, hydrological, and biological attributes and drivers (Moore et al. 2002; Sagerfors et al. 2008). The collection of high resolution, time-series NEE data (e.g., hourly) is often hindered by interference such as instrument failure and unfavorable weather, which lead to gaps in the data (Falge et al. 2001). These incomplete data sets ultimately reduce confidence in the scaled-up estimations of NEE (e.g., daily, weekly, monthly, seasonal, annual). A modeling approach can, however, compensate for limited or incomplete data collection, thereby providing more robust estimations of continuous fine-resolution NEE data.

The Florida Everglades is one of the largest subtropical wetlands in North America, encompassing an area in excess of 6000 km^2 (Jimenez et al. 2012). The wetland form and function is greatly influenced by wet and dry seasons, storm activity, fluctuations in water quality and quantity (water depth and flow rate), and forest fires. Previous research (e.g., Schedlbauer et al. 2010, 2011, 2012; Jimenez et al. 2012; Malone et al. 2014a, b) extensively focused on elucidating the hydroclimatic controls and inter-annual variability of

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NEE in the Everglades freshwater wetlands. Regression-based models were developed to explore the driver-response linkages without delving much into the predictive domain. Further, various empirical models were used to fill gaps in the continuous (e.g., half-hourly) time-series of observed NEE from Everglades wetlands as a part of the AmeriFlux network (Moffat et al. 2007). These empirical gap-filling methods include the site- and time-specific applications of mean diurnal variation (Falge et al. 2001), ambient environmental conditions based 'look-up' tables (Falge et al. 2001), and parametric/non-parametric statistical approaches such as the artificial neural networks and non-linear regressions (e.g., Papale and Valentini 2003; Hui et al. 2004; Stauch and Jarvis 2006; Moffat et al. 2010). However, applications of the current gap-filling models require a large set of observations for environmental variables and/or NEE as inputs, posing a challenge in estimating NEE with limited information.

Harmonic modeling offers a solution to the current shortcomings primarily because it only requires input data for the predictant itself. Further, a parsimonious harmonic model can provide predictions with a small set of parameters, thereby reducing the inherent model uncertainty (e.g., Abdul-Aziz et al. 2007; Abdul-Aziz and Ishtiaq 2014). Although the classical harmonic analysis (Priestley 1981) has been widely used to develop empirical models in numerous applications of environmental sciences and engineering (e.g., Nestler and Long 1997; Meyers et al. 2001; Dyar and Alhadeff 2005; Kumar et al. 2006), only a few studies applied harmonic functions for modeling NEE. However, the cyclic pattern of ecological/environmental variables such as NEE lends itself to the development of relatively simple, predictive empirical models from the Fourier (harmonic) series expansion (Priestley 1981). Griffis and Rouse (2001) utilized the fast Fourier transformation and power spectral analysis to predict the inter-annual variability of NEE for a northern peatland. Other studies (Hollinger et al. 2004; Richardson and Hollinger 2005) developed second order harmonic regression models to predict the nocturnal CO_2 fluxes from terrestrial ecosystems.

A common limitation of empirical modeling, however, is the time- and site-specificities of the estimated parameters. Spatial and temporal differences among datasets mean a model trained with data for one reference time and/or site cannot be directly applied to a different time and/or site, unless the model is recalibrated for the new scenario. The non-uniqueness of parameters remains as the major gap in empirical modeling of ecosystem carbon fluxes (Beer et al. 2010). Scaling has been widely used in environmental sciences and engineering to develop robust models by leveraging the underlying similarity among different references (e.g., Milne et al. 2002; Enquist et al. 2003; O'Connor et al. 2006; Warnaars et al. 2007; Hondzo and Warnaars 2008). Abdul-Aziz et al. (2007) presented a novel scaling approach to develop an extended stochastic harmonic analysis algorithm (ESHA), which can estimate stream dissolved oxygen (DO) at a chosen reference time (e.g., noon) from a single or multiple grab samples collected at any time of the diurnal cycle. Abdul-Aziz and Ishtiaq (2014) expanded the ESHA to develop a scaling-based empirical model that can robustly predict the entire diurnal cycles of stream DO for different days and sites from the corresponding single reference observations.

The objective of this study is to develop a scaling-based harmonic (i.e., ESHA) model to estimate the different diurnal cycles of hourly NEE for the Florida Everglades freshwater marshes using the day- and site-specific single or multiple reference measurements. The study builds on the hypothesis that scaling of the diurnal NEE cycles by the corresponding day- and site-specific single reference observations would lead to a general, dimensionless NEE cycle for all days and sites. Estimation of the generalized NEE cycle is expected to involve a single and parsimonious set of parameters, requiring only single reference observations to estimate the respective hourly NEE for different days, years, and sites. The empirical model is presented in user-friendly formats to aid the wetland scientists and managers in estimation and gap-filling of hourly NEE data for the Everglades freshwater wetlands.

Materials and Methods

The Scaling-Based Harmonic Model Theory

A conceptual illustration of the scaling-based harmonic modeling theory is made by using a schematic of several hypothetical diurnal cycles of NEE to represent different (1, 2, ….., N) days for a single or multiple wetland sites (Fig. 1a). An un-scaled harmonic model would ideally require N unique sets of parameter values to represent the N diurnal cycles of NEE. In contrast, the scaling-based ESHA can lead to a single set of model parameters across different days and sites. The ESHA scales (i.e., normalizes) each diurnal cycle by a corresponding reference time (t_{ref}) single observation, NEE_{ref}. The scaling would lead to a collapse of different NEE cycles on a generalized, dimensionless diurnal NEE cycle (NEE^*) with a value of NEE^*_{ref} at t_{ref} (Fig. 1b). The scaled NEE cycle flips to a convex shape since the original (concave) diurnal cycles (Fig. 1a) are normalized by a daylight time, negative reference NEE. The scaled model (NEE^*) is then estimated with the ESHA parameterization framework (see 'Estimation of the ESHA Model Parameters' for details) using observed time-series of NEE. The dimensionless model is ideally robust because it represents all (i.e., N) predicted days at the same or similar sites with a single set (instead of N sets) of

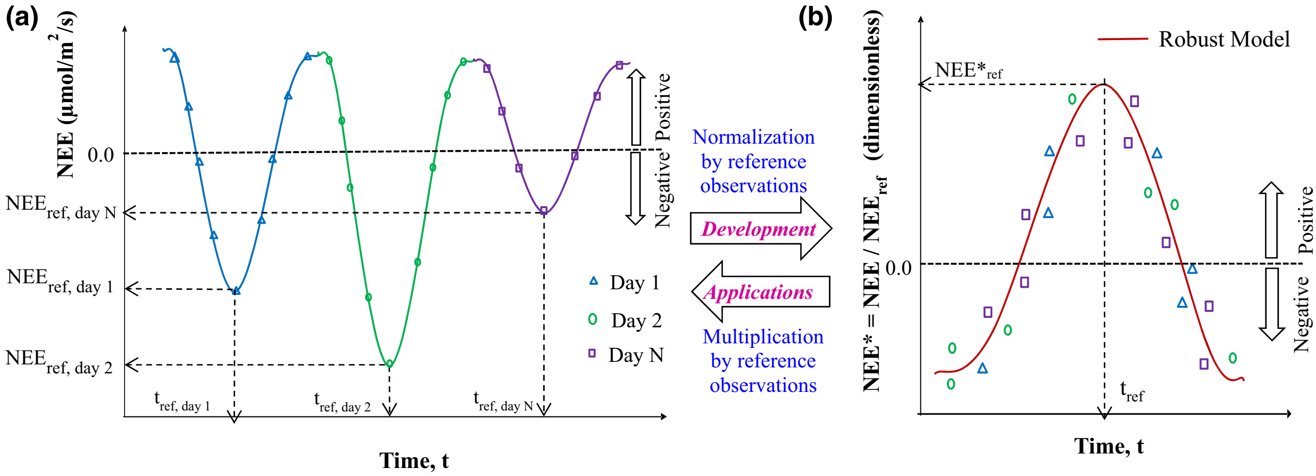


Fig. 1 Conceptual framework for (**a**) development and (**b**) application of the scaling-based net ecosystem exchange (NEE) model for Everglades freshwater wetlands

parameters. The different day-specific NEE cycles are then obtained by multiplying the estimated dimensionless NEE^* model by the corresponding single reference observations, NEE_{ref}.

Estimation of the ESHA Model Parameters

The mathematical framework of ESHA was originally developed and presented in details by Abdul-Aziz et al. (2007). Therefore, the ESHA framework is briefly but adequately stated here for parameter estimations. A stochastic Fourier series, $y(t)$ (Priestley 1981) is defined as

$$y(t) = a_0 + \sum_{k=1}^{W} \left[a_k \cos(2\pi f_k t) + b_k \sin(2\pi f_k t)\right] + \varepsilon(t) = h(t) + \varepsilon(t) \quad (1)$$

where $y(t)$ = periodic response variable = $NEE^*(t)$ (see Fig. 1b), t = predictor variable = time, k = harmonic number, W = optimum number of harmonics necessary to represent the wave frequencies and components of a diurnal cycle of NEE, a_0 = non-oscillatory ($k = 0$) model component, a_k and b_k = Fourier coefficients associated with the oscillatory components of the harmonic series, $f_k = \frac{k}{n\Delta t} = k^{\text{th}}$ harmonic frequency, n = total number of observations within a 24-h diurnal cycle (i.e., $n = 24$), Δt = sampling interval (e.g., 1 h), $\varepsilon(t)$ = random error, and $h(t) = y(t) - \varepsilon(t)$ is the harmonic process. Unlike a classical harmonic analysis (Priestley 1981), the ESHA forces the harmonic process $h(t)$ to pass through a known value κ, which is the NEE^* observation at the reference time (t_{ref}). This forcing leads to a "zero" prediction error at t_{ref} for individual cycle; i.e., $\varepsilon(t_{ref}) = 0$, and $h(t_{ref}) = y(t_{ref}) = \kappa = NEE^*(t_{ref}) = NEE^*_{ref}$. The non-oscillatory model component parameter, a_0 is then derived from Eq. (1) as follows:

$$a_0 = \kappa - \sum_{k=1}^{W} \left[a_k \cos\left(2\pi f_k t_{ref}\right) + b_k \sin\left(2\pi f_k t_{ref}\right)\right] \quad (2)$$

First, the parameters of the oscillatory model components (a_k, b_k; $k = 1, 2, \ldots, W$) are estimated using a least-squares error minimization method from a system of equations as follows:

$$P = Q^{-1} R \quad (3)$$

where P = parameter (i.e., $\hat{a}_k, \hat{b}_k$ for $k \neq 0$ with 'hat' representing estimation) vector of length $2W$, $Q = 2W \times 2W$ non-singular transition matrix, and R = vector of length $2W$ with terms associated with any observations $y(t) = NEE^*(t)$ and the reference-time observation $\kappa = NEE^*(t_{ref})$. The parameter $\hat{a}_0$ is then computed from Eq. (2). An explicit form of Eq. (3) for two harmonics (i.e., $W = 2$) is presented in the Supplemental notes (Eq. S1) as examples.

The main difference between a classical harmonic analysis and the ESHA is in their parameter estimations. ESHA provides the correct parameter estimation framework to force the harmonic model through a reference-time normalized observation. The forcing, in turns, allows a proper estimation of the entire diurnal cycle of NEE from a single reference observation.

The ESHA Modeling Steps

Step 1: *Collection of hourly NEE data, NEE(t) for multiple 24-h diurnal cycles*

Development of the scaling-based ESHA model requires continuous (e.g., hourly) NEE data for at least one (and preferably for multiple) 24-h diurnal cycle(s) for a single or multiple wetland sites. The model application requires at least a single reference-time observation to predict the corresponding diurnal cycle. The hourly NEE for two Everglades wetlands were collected from AmeriFlux (2016), which represents flux tower based eddy-covariance measurements (see 'Case Study Wetlands' and 'Datasets' for details).

Step 2: *Selection of a reference-time (t_{ref}) observation, $NEE_{ref} = NEE(t_{ref})$ for each cycle*

In theory, the ESHA framework allows the selection of any diurnal hour as t_{ref} and the corresponding NEE observation as the reference observation for scaling the respective diurnal cycle. However, a negative NEE (i.e., daylight time net uptake flux) has to be chosen as reference observation to obtain a consistently convex shape of the scaled NEE (see Fig. 1). To select the optimum reference time-window, a user needs to test model performance (e.g., explanation of variance in NEE data) by estimating the diurnal cycles using different daytime hours as a reference time. It is recommended to test the optimization for each hour between 8:00 A.M. and 4:00 P.M. since this time-window typically represents the peak photosynthesis and the maximum magnitude of negative NEE. The daytime hours showing a superior model performance within the tested time-window should be used as the reference times.

Step 3: *Normalizing (*i.e.*, scaling) of individual NEE cycles*

Each NEE cycle is then normalized by the corresponding day-specific reference observation (NEE_{ref}) to obtain a dimensionless NEE cycle as follows (see 'The Scaling-Based Harmonic Model Theory' and Fig. 1): $NEE^*(t) = NEE(t)/NEE_{ref}$.

Step 4: *Estimating the normalized diurnal cycles of NEE by employing ESHA*

Each normalized NEE cycle, $NEE^*(t)$ is then fitted by applying the ESHA parameter estimation framework (see 'Estimation of the ESHA Model Parameters') to force each cycle through the reference-time normalized observation, $NEE^*(t_{ref}) = NEE(t_{ref})/NEE_{ref} = 1.0 = \kappa$. In case of multiple diurnal cycles, such fitting should result in a set of estimate parameters, where each parameter set represents a diurnal cycle.

Step 5: *Obtaining a generalized (*i.e.*, robust) scaled model, $NEE^*_{\mathrm{mod}}(t)$*

The estimated parameters of the scaled, dimensionless cycles for all available days should ideally be robust in space and time. Ensemble averages of the model parameters over time are computed for each site to obtain the temporally generalized model for that site. A spatiotemporally generalized model is then obtained by averaging the parameters from different sites and days.

Step 6: *Estimating the individual diurnal cycles*

The individual 24-h diurnal cycles, $NEE_{\mathrm{mod}}(t)$ is then estimated by multiplying the generalized scaled model, $NEE^*_{\mathrm{mod}}(t)$ — developed from the site-specific temporally ensemble and/or spatiotemporally ensemble parameter set — by the corresponding single reference observations (NEE_{ref}) as follows (see Fig. 1):

$$NEE_{\mathrm{mod}}(t) = NEE_{ref} \times NEE^*_{\mathrm{mod}}(t) \quad (4)$$

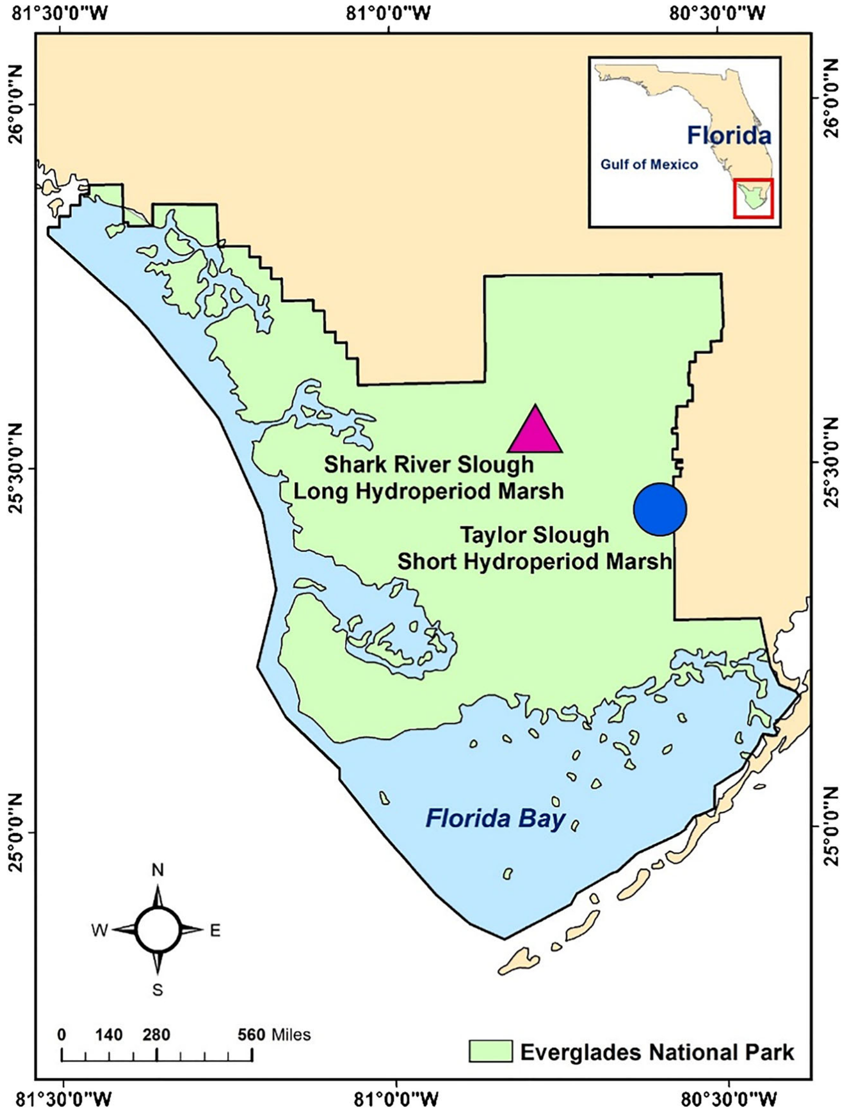
Quantification of Model Sensitivity and Uncertainty

Mathematical modeling and parametrizations of environmental and ecological systems is inherently uncertain. Therefore, a quantification of the model sensitivity and uncertainty is useful to determine confidence associated with the predictions. The ESHA model sensitivity to any changes in an individual parameter was determined by analytically deriving dimensionless sensitivity coefficients (see Eqs. S2–S4 and details in Supplemental notes). Model uncertainty to simultaneous changes in all parameters by their respective standard deviations was quantified by deriving the corresponding standard deviation of predicted NEE (Eq. S5).

Case Study Wetlands

The study wetlands are located inside the Everglades National Park and represent the sites of the Florida Coastal Everglades Long Term Ecological Research (FCE LTER 2016). Subject to the availability of year-round hourly eddy-covariance observations, two oligotrophic freshwater marshes were selected for model evaluations: a short-hydroperiod marsh located in Taylor Slough (25°26′16.50″N, 80°35′40.68″W), and a long-hydroperiod marsh located in Shark River Slough (25°33′6.72″N, 80 °46′57.36″W) (Fig. 2). Much details into the hydrological, ecological, biogeochemical, and biological characteristics of the two marshes can be found in Schedlbauer et al. (2012). In general, Florida Everglades is characterized by a subtropical climate, well-defined wet and dry seasons (wet: November–May; dry: June–October), and year-round productivity (Obeysekera et al. 1999; Ewe et al. 2006). Hydrology of the two wetlands is extensively managed (USACE and SFWMD 1999), with water flows controlled by a combination of pumping and constructed levees. The Taylor Slough marsh site experiences seasonal flooding for approximately four to six months (June – November) per year (Malone et al. 2014a, b). Sawgrass (*Cladium jamaicense*) and C4 muhly grass (*Muhlenbergia capillaris*) are the prevailing vegetations and primary producers at this site; periphyton and submerged macrophytes are also known to geochemically fix CO_2 (as $CaCO_3$) during flooding seasons (Schedlbauer et al. 2010, 2012). In contrast, the Shark River Slough marsh site experiences year-round inundation due to a ridge-slough topography. The vegetation is dominated by *Cladium jamaicense*, *Eleocharis*

Fig. 2 Locations of the two study wetlands within the Everglades National Park



sp., emergent *Panicum sp.*, and submerged *Ultricularia sp*. The soil type is marl at Taylor Slough and deposited pit at Shark River Slough, as characterized with overlying limestone bedrock in both sites.

Datasets

The hourly 'with-gap' (i.e., un-filled) NEE (μmol/m^2/s) observations (level − 2) for the two Everglades wetlands were collected from AmeriFlux (2016). The hourly data were subsampled from the 30-min average time-series for 24-h diurnal cycles (starting at 1:00 AM) during 2008–2013 (Taylor Slough: 2008–13, and Shark River Slough: 2009–13). In addition, the corresponding data for photosynthetically active radiation (PAR, μmol/m^2/s), air temperature (TA, ^{o}C), water level (WL, cm), total nitrogen (μmol/l), and total phosphorous (μmol/l) were obtained from AmeriFlux (2016) and FCE LTER (2016) to investigate any relationships between the model parameters and the major ecohydrological and environmental drivers of wetland NEE at the study sites.. We followed the standard AmeriFlux sign conventions, where negative NEE indicates the downward (atmosphere to wetland) fluxes and positive NEE represents the upward (emissions to the atmosphere) fluxes.

Modeling with AmeriFlux data can be significantly impacted by measurement errors and uncertainty (Williams et al. 2009; Schmidt et al. 2012). We applied five data-screening steps to ensure a good quality of data used for this research. First, the nighttime friction velocity (u*) threshold for each year was determined based on Aubinet et al. 2012 (see Supplemental notes for details), and the hourly NEE representing lower u* values (i.e., low turbulence conditions) were removed. Second, the extreme values or outliers in NEE were identified and removed based on thresholds obtained by using year-specific 1st and 99th percentile values of NEE. The extreme percentiles criteria was found to be the most effective and realistic (least exclusive) method in detecting outliers of the hourly NEE time-series among other acceptable statistical methods (e.g., inter-quartile range, confidence intervals). Third, unreasonable spikes in the hourly time-series were filtered by using a variant of the central difference method described in Papale et al. (2006) (see Eqs. S6-S8 and details in Supplemental notes). Fourth, occasional diurnal cycles were excluded when $NEE_{ref} > -1$ μmol/m^2/s for a chosen reference time (t_{ref}) to ensure a consistently convex shape of the scaled diurnal cycle (see Fig. 1b; details are given in 'Choice of Reference Time'). Fifth, to avoid model bias toward any outlying diurnal cycles, the outlying daily estimates of each parameter were identified by applying the respective inter-quartile range (IQR) criteria (Tukey 1977). Any daily parameter value outside the range between Q_1–2*IQR and Q_3 + 2*IQR (here, Q_1 = first quartile, Q_3 = third quartile, and IQR = Q_3-Q_1) were removed from further analysis along with the corresponding diurnal cycle of NEE.

As ESHA model parameterization requires all 24 hourly observations of NEE for a day, the screened calibration data sets were gap-filled using linear interpolations (from *interpl* command in Matlab). However, we considered only those diurnal cycles for interpolations that had four or less consecutive hourly gaps to limit any biases arising from the gap-filling. Finally, the QA/QC methods provided up to 55 and 69 complete diurnal cycles for model parameter estimations and calibrations, respectively, for Taylor Slough during 2008–11 and for Shark River Slough during 2009–11 (see Table 1 and 2). The remaining, independent two years (2012–13) of filtered data were used for model validations at each site. However, it was not necessary to filter the validation datasets for any outlying diurnal cycles based on the outlying parameters, which had already been estimated with the calibration data. Further, unlike the calibration datasets, the validation data were not gap-filled as model validation does not require 24-h continuous measurements of NEE. Consequently, a larger number of incomplete diurnal cycles (173–262; see Table 3) were available during 2012–13 for model validations, compared to the number of complete cycles for calibrations (Table 2) during 2008–11. A successful validation will, therefore, indicate the utility of the calibrated models to estimate the entire diurnal cycles from the limited available data, which is often the case for most sampling days.

Results and Discussion

Model Optimization

Optimal Number of Harmonics

Selection of the optimal number of harmonics (*W*) provides a crucial balance between model parsimony (a minimum number of parameters) and accuracy. Following Abdul-Aziz and Ishtiaq (2014), a dimensionless Akaike Information Criterion

Table 1 Data summary of NEE, and the climatic and environmental variables used for model calibrations at the two Everglades wetlands. Statistics of NEE and the associated years for validations are given in parenthesis

Sites	Years	Statistics	NEE (μmol/m^2/s)	PAR (μmol/m^2/s)	Air Temperature (°C)	Water Level (cm)	Total Phosphorous Concentration (μmol/l)	Total Nitrogen Concentration (μmol/l)
Taylor Slough short hydroperiod marsh	Calibration: 2008–11 (2012–13)	Mean	−0.18 (−0.85)	408.59	23.12	55.51	0.20	51.63
		Standard deviation	1.44 (1.62)	139.94	5.27	32.62	0.21	37.82
		Maximum	2.50 (2.53)	656.03	31.45	102.78	2.1	215.26
		Minimum	−4.42 (−5.56)	139.55	9.48	0	0	11.81
Shark River Slough long hydroperiod marsh	Calibration: 2009–11 (2012–13)	Mean	−0.13 (−0.28)	418.85	21.27	45.54	0.25	123.91
		Standard deviation	1.12 (1.01)	136.52	7.20	11.72	0.13	119.60
		Maximum	2.36 (1.90)	700.75	32.54	78.56	1.02	1005.89
		Minimum	−3.98 (−3.18)	151.08	8.01	25.43	0.03	13.85

Table 2 Site-specific and generalized sets (temporal and spatiotemporal averages, respectively) of estimated parameters over the calibration periods (2008–11) for the two Everglades wetlands

Site	Reference time (hour of the day)	Number of predicted days	$\hat{a}_0$	$\hat{a}_1$	$\hat{a}_2$	$\hat{b}_1$	$\hat{b}_2$	NSE	RSR
Taylor Slough short hydroperiod marsh (2008–11)	8	24	0.35 (0.10)	−1.32 (0.50)	0.19 (0.19)	0.02 (0.19)	−0.08 (0.13)	0.77	0.47
	9	42	0.22 (0.09)	−1.02 (0.25)	0.24 (0.16)	−0.01 (0.16)	−0.07 (0.12)	0.84	0.40
	10	47	0.16 (0.08)	−0.84 (0.16)	0.27 (0.13)	−0.06 (0.14)	−0.01 (0.10)	0.85	0.38
	11	55	0.11 (0.09)	−0.74 (0.11)	0.23 (0.11)	−0.06 (0.11)	0.03 (0.10)	0.87	0.36
	12	55	0.09 (0.11)	−0.71 (0.10)	0.20 (0.11)	−0.07 (0.12)	0.02 (0.09)	0.88	0.36
	13	52	0.08 (0.12)	−0.74 (0.10)	0.20 (0.12)	−0.06 (0.11)	0.02 (0.09)	0.88	0.36
	14	46	0.12 (0.11)	−0.80 (0.09)	0.25 (0.13)	−0.06 (0.12)	0.03 (0.10)	0.89	0.33
	15	44	0.17 (0.12)	−0.96 (0.15)	0.28 (0.17)	−0.13 (0.10)	0.06 (0.12)	0.88	0.34
	16	35	0.23 (0.13)	−1.11 (0.22)	0.22 (0.17)	−0.21 (0.11)	0.16 (0.14)	0.87	0.37
Shark River Slough long hydroperiod marsh (2009–11)	8	27	0.23 (0.18)	−1.02 (0.31)	0.04 (0.18)	0.12 (0.22)	−0.20 (0.12)	0.65	0.59
	9	44	0.19 (0.15)	−0.98 (0.30)	0.17 (0.22)	0.01 (0.24)	−0.10 (0.15)	0.67	0.58
	10	63	0.12 (0.15)	−0.86 (0.20)	0.22 (0.22)	−0.03 (0.25)	−0.04 (0.16)	0.71	0.54
	11	64	0.12 (0.11)	−0.76 (0.15)	0.21 (0.16)	−0.08 (0.21)	0.02 (0.14)	0.76	0.49
	12	69	0.10 (0.12)	−0.72 (0.14)	0.18 (0.14)	−0.09 (0.21)	0.02 (0.13)	0.76	0.48
	13	54	0.12 (0.12)	−0.69 (0.13)	0.19 (0.13)	−0.12 (0.16)	0.03 (0.12)	0.80	0.45
	14	43	0.14 (0.10)	−0.71 (0.12)	0.22 (0.11)	−0.14 (0.14)	0.07 (0.10)	0.84	0.41
	15	43	0.18 (0.10)	−0.84 (0.17)	0.23 (0.13)	−0.18 (0.15)	0.10 (0.13)	0.82	0.42
	16	44	0.23 (0.13)	−0.99 (0.24)	0.20 (0.21)	−0.29 (0.16)	0.14 (0.14)	0.75	0.50
Generalized	*11–14*		*0.11*	*−0.74*	*0.21*	*−0.09*	*0.03*		

(1) Values in parentheses are the standard deviations of the estimated parameters. (2) NSE = Nash-Sutcliffe Efficiency; RSR = ratio of root-mean-square error (RMSE) to the standard deviations of observations. NSE and RSR, respectively, indicate the goodness-of-fit and accuracy of the model

Table 3 Results of model validation using the site-specific parameters and the generalized parameters (in parentheses) for the different reference times (11 A.M. to 2 P.M.) during 2012–13

Sites	Reference time (hour of the day)	Number of validation days	NSE	RSR
Taylor Slough	11	253	0.77 (0.78)	0.48 (0.47)
	12	255	0.77 (0.78)	0.48 (0.47)
	13	262	0.76 (0.78)	0.49 (0.47)
	14	241	0.76 (0.76)	0.49 (0.49)
Shark River Slough	11	209	0.66 (0.67)	0.58 (0.58)
	12	184	0.71 (0.71)	0.54 (0.54)
	13	177	0.74 (0.74)	0.51 (0.51)
	14	173	0.72 (0.72)	0.53 (0.53)

NSE = Nash-Sutcliffe Efficiency; RSR = ratio of root-mean-square error (RMSE) to the standard deviations of observations. NSE and RSR, respectively, indicate the goodness-of-fit and accuracy of the model

(AIC) (Akaike 1974) (see Eq. S9 and details in Supplemental notes) was computed by incorporating up to 12 harmonics using the calibration data assuming mid-point of the day (12 P.M.) as the reference time (Fig. 3a). The minimum AIC indicated the most accurate and optimal model. For Shark River Slough, a total of two harmonics ($W = 2$) apparently resulted in the minimum AIC, leading to a five parameter model (number of parameter, $P = 2W + 1$). For Taylor Slough, $W = 2$ increased the model accuracy (decreased AIC) by 15% compared that for $W = 1$. However, $W = 3$ increased the model accuracy by only 3% for a 40% increase in the number of parameters compared to that for $W = 1$. Therefore, $W = 2$ was selected as the optimal number of harmonics for both sites as a compromise between model parsimony and prediction accuracy, leading to the estimation of five model parameters ($\hat{a}_0$, $\hat{a}_1$, $\hat{b}_1$, $\hat{a}_2$, and $\hat{b}_2$) for each wetland. The two-harmonic model also reflects a mechanistic basis. The $\hat{a}_0$ represents the daily quasi-mean of NEE^*; the first harmonic parameters ($\hat{a}_1$, $\hat{b}_1$) represent the primary frequency components of the diurnal oscillations, whereas the second harmonic parameters ($\hat{a}_2$, $\hat{b}_2$) incorporate the secondary (e.g., seasonal) frequency components embedded in a diurnal cycle.

Choice of Reference Time

Based on the calibration datasets (Table 1), the impact of using different reference times on the two-harmonic model performance was shown for a set of daytime hours (e.g., 8:00 A.M. to 4:00 P.M.) (Fig. 3b). For each reference time, occasional diurnal cycles were excluded if the corresponding $NEE_{ref} > -1$ μmol/m^2/s to preserve the convex shape of the scaled NEE model, while including all NEE > −1 μmol/m^2/s values for the other 23 h. The model performance was measured by Nash-Sutcliffe Efficiency (NSE) that is similar to the coefficient of determination (R^2) (Eq. S10 in Supplemental notes), where NSE = 1.0 indicates a perfect model. As shown (Fig. 3b), the 8–16 h time-window (i.e., 8:00 A.M. to 4:00 P.M.) provided an acceptable model performance (NSE ≥ 0.65) for both study sites — indicating the flexibility for selecting any time between 8 and 16 h of a diurnal cycle as the reference time. However, model performance was stronger for choosing a reference time between 10 A.M. and 4 P.M. (NSE > 0.70 for Shark River and NSE > 0.80 for Taylor Slough).

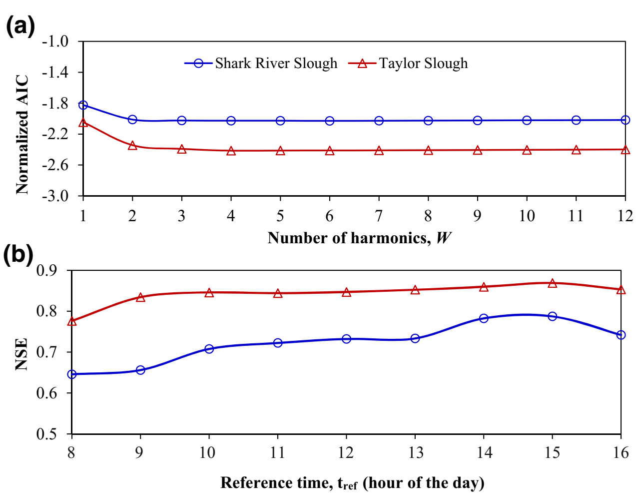


Fig. 3 Selection of the optimal (**a**) number of harmonics and (**b**) reference time for the harmonic NEE model. Akaike Information Criteria (AIC) indicates model accuracy and Nash-Sutcliffe Efficiency (NSE) indicates the goodness of model fitting

Estimation and Generalization of Model Parameters in Time and Space

The five parameters ($\hat{a}_0$, $\hat{a}_1$, $\hat{b}_1$, $\hat{a}_2$, and $\hat{b}_2$) of the ESHA model were estimated with the calibration datasets for individual diurnal cycles by using each hour from 8 A.M. to 4 P.M. (8–16 h) as the reference time, separately. The spatiotemporal trends of model parameters were explored by plotting their day-specific estimates with the corresponding Julian days for the two Everglades marshes. For example, the plots of Julian days versus model parameters across sites for the mid-day (12 P.M.) reference time (i.e., t_{ref} = 12 h) were shown (Fig. 4). The model parameters did not show any predictable increasing or decreasing trends (NSE and slope of linear regression of parameters with the Julian days ranged from 0.005 to 0.023, and 0.000007 to 0.0002, respectively) over the calibration period, despite the slight sag of $\hat{a}_1$ and $\hat{a}_2$ during the summer-growing season (Julian days = 130–273) — indicating the temporal robustness of the model parameters. The plots also suggested a spatiotemporal robustness of the model parameters as they collapsed into comparable ranges between the two sites. The closeness of the parameters among different days and sites were further evaluated by computing the index of dispersion, D, which is the ratio of the parameter variance to the respective absolute mean (Cox and Lewis 1966; Upton and Cook 2006). D = 0 indicates a perfectly constant variable, 0 < D < 1 indicates under-dispersion, and D > 1 indicates over-dispersion. The relatively small D values (0.13, 0.02, 0.09, 0.38, and 0.52 for $\hat{a}_0$, $\hat{a}_1$, $\hat{b}_1$, $\hat{a}_2$, and $\hat{b}_2$, respectively) clearly indicated an under-dispersion of the parameters among the different days and sites.

The relationships between the model parameters and the major drivers of wetland NEE were investigated to achieve further insights into the spatiotemporal robustness of estimated parameters. As examples, the daily estimates (for t_{ref} = 12 h) of the principal parameter, $\hat{a}_0$ were plotted with the corresponding daily average of photosynthetically active radiation, air temperature, and water level for both study sites (Fig. 5). The plotted parameters did not display any predictable trends with the ecohydrological drivers across the two wetlands. Further, the non-oscillatory parameter, $\hat{a}_0$ did not

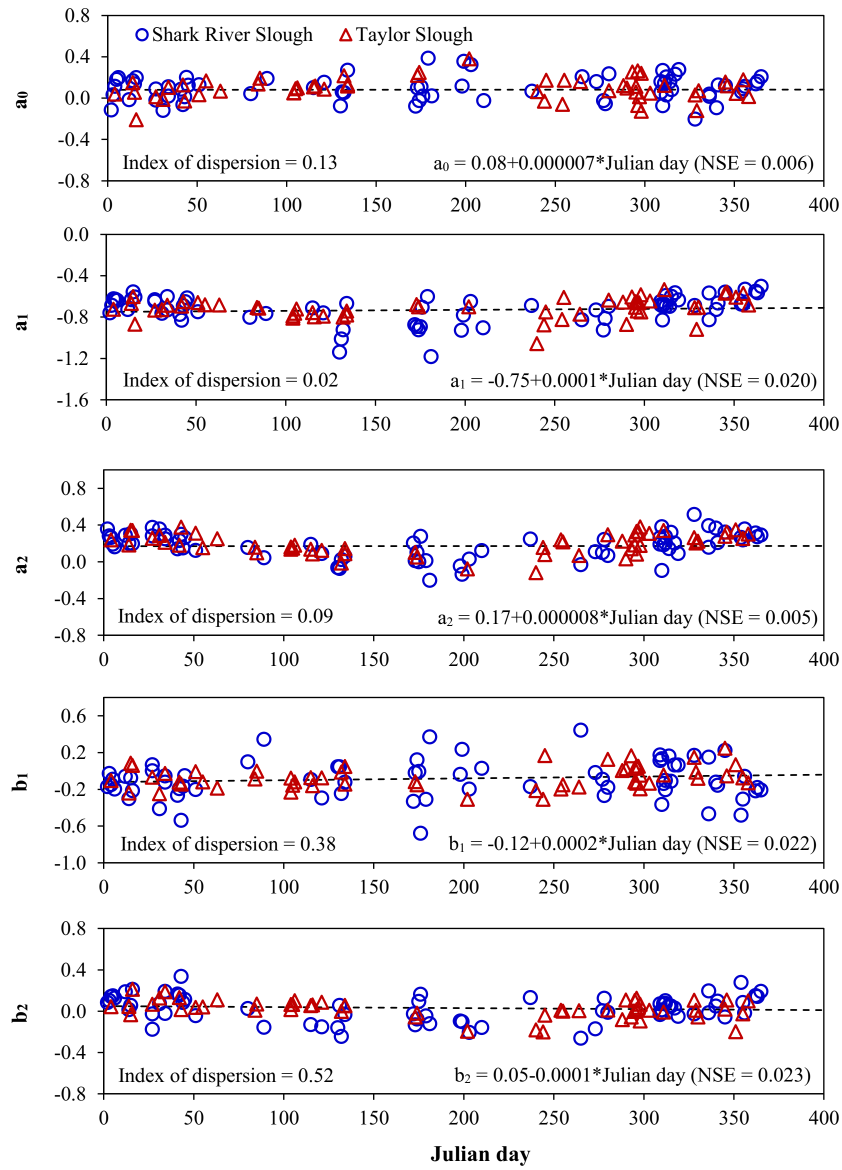


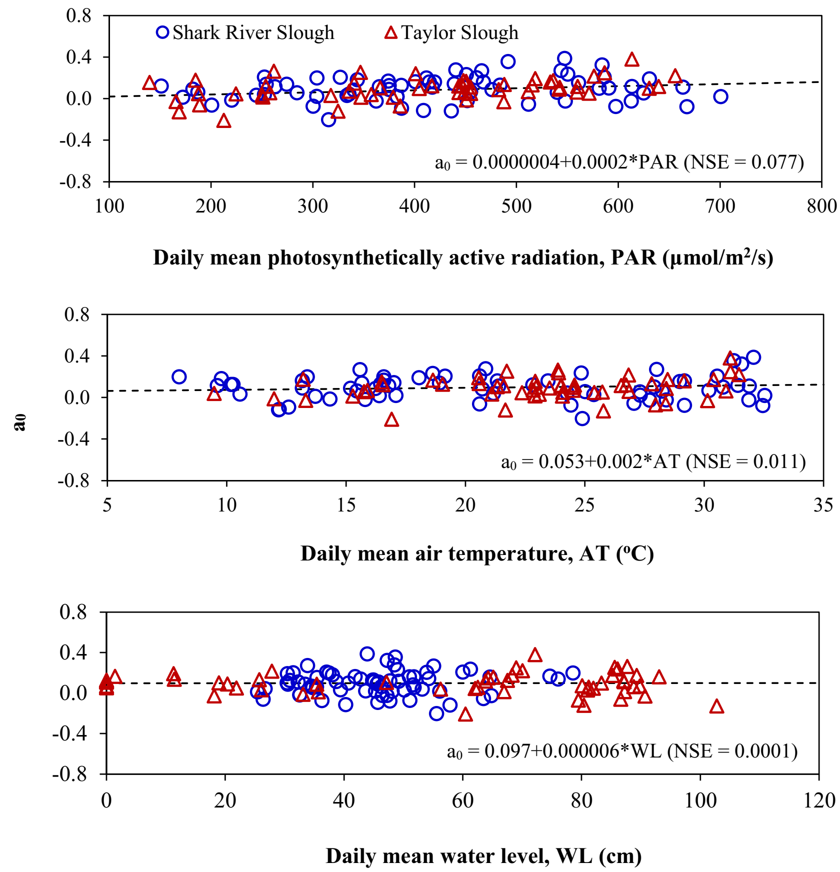
Fig. 4 Daily estimates of the model parameters with the Julian days of the calibration period (2008–11) for the Everglades wetlands, using noon (12 P.M.) as the reference time (i.e., t_{ref} = 12 h). The dotted (black) line indicates the trend line. The equations were obtained from linear regressions of model parameters with Julian days

show any apparent sensitivity to the daily fluctuations of total nitrogen and phosphorus concentrations (see Fig. S1 in Supplemental notes).

Given the notable invariance of model parameters in time, the site-specific (temporal) ensemble sets of parameters for each t_{ref} were obtained by averaging the respective daily estimates over all seasons and years of the calibration periods (Table 2). The temporal ensembles suggested comparable parameter values within the reference time window of 11 A.M. to 2 P.M. (i.e., t_{ref} = 11 to 14 h) across the two marshes. For example, the temporal means of the major model parameter $\hat{a}_0$ for Taylor Slough ranged from 0.08 to 0.12, which were similar to that of $\hat{a}_0$ (0.10 to 0.14) for Shark River Slough. The corresponding ranges of the first harmonic parameters ($\hat{a}_1 = -0.69$ to -0.80; $\hat{b}_1 = -0.06$ to -0.14) and the second harmonic parameters ($\hat{a}_2$ = 0.18 to 0.25; $\hat{b}_2$ = 0.02 to 0.07) were also similar between the two sites. A generalized, single set of model parameters in time and space was, therefore, obtained by averaging the respective parameters estimated with each reference time during 11–14 h for both sites (Table 2, last row).

The observed robustness of estimated model parameters in time and space was achieved by the application of scaling; normalization of each diurnal NEE cycle by the corresponding single reference observation brought parameters of different days, years and sites into comparable ranges. The temporal robustness of the model parameters suggests that the site-specific ensemble (temporally averaged) sets of parameters will result temporally robust estimations of hourly NEE from a reference time observation made during 8 A.M. to 4 P.M. (Table 2). Based on the similarity of parameters among the four

Fig. 5 Daily estimates of the principal model parameter, $\hat{a}_0$ with the corresponding mean photosynthetically active radiation, air temperature, and water level for the calibration days during 2008–11 at the Everglades wetlands, using noon (12 P.M.) as the reference time. The dotted (black) line indicates the trend line. The equations were obtained from linear regressions of $\hat{a}_0$ with the ecohydrological drivers



reference times across the two marshes (Table 2), the generalized single parameter set would also lead to good quality (i.e., spatiotemporally generalized) estimations of NEE cycles from any reference observation made during 11 A.M. to 2 P.M.

Evaluation of the Site-Specific Models

The site-specific temporally averaged (over the calibration period) parameters (Table 2) for different reference times during 11 A.M. to 2 P.M. were used to simulate the hourly NEE cycles from the corresponding day-specific reference observations for both study wetlands. Model evaluation with the calibration data sets showed very good fitting efficiency (NSE = 0.87–0.89) and accuracy (ratio of root-mean-square-error to the standard deviation of observations, RSR = 0.33–0.36) with different t_{ref} for Taylor Slough (Table 2) (see Eqs. S10–S11 in Supplemental notes for details on NSE and RSR). The model also showed good performance for the Shark River Slough (NSE = 0.76–0.84; RSR = 0.41–0.49). The observed versus predicted hourly NEE (using t_{ref} = 12 h as an example) for both wetlands were shown in scatter-plots (Fig. 6).

The temporally averaged site-specific parameters of each reference time during 11 A.M. to 2 P.M. were used to validate the harmonic model for the corresponding site with 173–262 incomplete diurnal cycles of hourly NEE observations from two independent years (2012–13). The site-specific model validations showed acceptable prediction performance

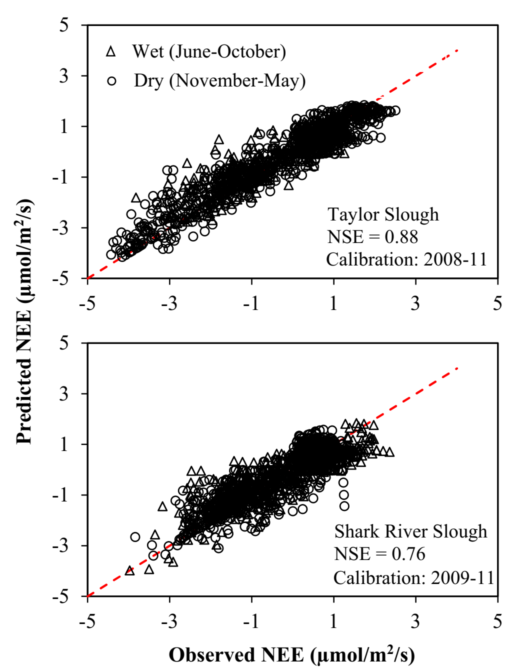


Fig. 6 Hourly observed vs. predicted NEE for calibrations during 2008–11 at the Everglades wetlands using the temporally ensemble means of site-specific model parameters for the noon (12 P.M.) reference time. Dotted line indicates the 1:1 line

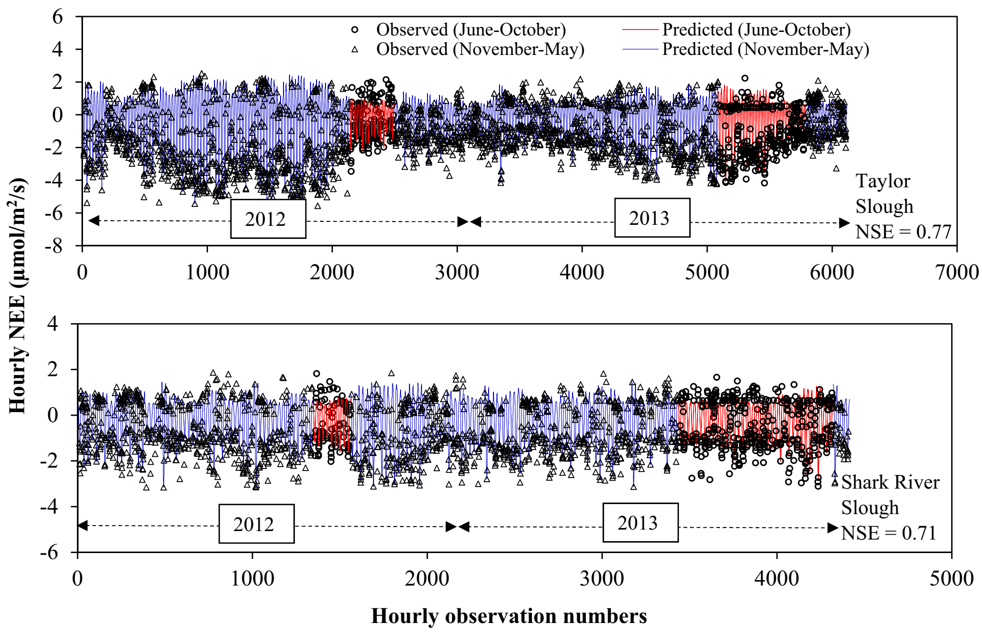


Fig. 7 Hourly time-series of observed and predicted NEE during the validation periods (20012–13) for the two Everglades wetlands using the site-specific temporally ensemble parameters for the noon (12 P.M.) reference time

(NSE = 0.66–0.77; RSR = 0.48–0.58) across the two wetlands (Table 3; Fig. 7). Furthermore, parameters estimated for one site (e.g., Shark River) were used to predict the hourly NEE for the other site (e.g., Taylor Slough) and vice versa to perform inter-site cross-validations during 2012–13. The validation results were similar to the site-specific validations (Table S1 in Supplemental notes). Overall, the model calibrations and validations demonstrated a unique ability of the scaling-based ESHA model to estimate the entire diurnal cycles of hourly NEE from the day- and site-specific single reference observations.

Performance of the Generalized Model

The model with the generalized parameter set was tested for each reference time between 11 A.M. and 2 P.M. with the validation datasets of both marshes. The generalized model resulted in similar fitting efficiency and accuracy (NSE = 0.67–0.78; RSR = 0.47–0.58), compared to that of the site-specific validations (Table 3; Fig. S2 in Supplemental notes). The success in simulating many independent, incomplete diurnal cycles of hourly NEE during 2012–13 — by using a single parameter set estimated with much fewer complete diurnal cycles during 2008–11 (Table 2) — shows robustness of the presented model across the two different wetlands. The results also indicate the potential utility of scaling for developing generalized modeling tools across different ecological and engineering disciplines.

Model Sensitivity and Uncertainty

The dimensionless sensitivity coefficient for $\hat{a}_0$ was 1.0 at all diurnal hours — indicating a constant and linear rate of change in the estimated NEE for any changes of $\hat{a}_0$ (Fig. S3 in Supplemental notes). However, the harmonic parameters ($\hat{a}_1$, $\hat{b}_1$, $\hat{a}_2$, and $\hat{b}_2$) showed dynamic sensitivities with the diurnal hours because of the presence of sine-cosine functions in their formulations. Among the 24 diurnal hours, sensitivity coefficients of the first harmonic parameters of $\hat{a}_1$ and $\hat{b}_1$ varied from 0 to 2 and −1 to 1, respectively; the second harmonic parameters of $\hat{a}_2$ and $\hat{b}_2$ varied from −2 to 0 and −1 to 1, respectively.

For illustration purpose, the model sensitivity and uncertainty were calculated by using t_{ref} = 12 h and the corresponding reference observations (NEE_{ref}) as examples. The average NEE_{ref} at 12 P.M. over the calibration periods for Taylor and Shark River Sloughs were −2.39 and −1.85 μmol/m^2/s, respectively. Based on Eq. S2, changing $\hat{a}_0$ by the corresponding standard deviations (see Table 2) resulted in a change of 0.22 to 0.26 μmol/m^2/s in the predicted NEE across the two sites. Separate changes in $\hat{a}_1$, $\hat{b}_1$, $\hat{a}_2$, and b_2 by their respective standard deviations (Eqs. S3–S4) led to absolute changes of the predicted NEE by up to 0.48 to 0.52, 0.29 to 0.39, 0.52 to 0.53, and 0.22 to 0.24 μmol/m^2/s, respectively. The simultaneous changes in all parameters by their standard deviations (Eq. S5) resulted in the standard deviations of the predicted NEE between −0.74 and −0.22 μmol/m^2/s for different diurnal hours across the two marshes (Fig. 8). Since the harmonic model was forced through the reference observation, the uncertainty was minimum at the example reference time (t_{ref} = 12 h), while increasing at hours that are farther away from the reference time.

How to use the Model?

Subject to the users' preferences, the developed model can be used to estimate the diurnal cycle of hourly NEE at both

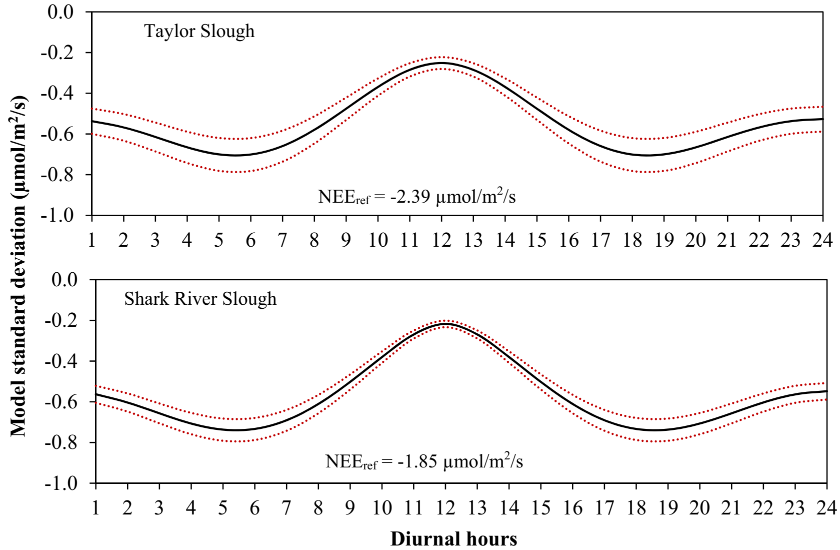


Fig. 8 Standard deviation of the predicted hourly NEE for simultaneously changing all parameters by their standard deviations at the Everglades wetlands. The solid (black) lines indicate the standard deviations computed by using the mean reference observation (NEE_{ref}) collected at 12 P.M. during the calibration period (2008–11). The dashed (red) lines refer to the standard deviations computed by using the 95% confidence limits of NEE_{ref}

Taylor and Shark River Sloughs from a corresponding single reference observation (collected during 11 A.M. to 2 P.M.) by utilizing any of the following tools: (I) Graphical approach, (II) the final model equation, or (III) the attached Excel spreadsheet model. If multiple reference observations of NEE are available during 11 A.M.-2 P.M. for the same diurnal cycle, we recommend using each reference observation separately to predict the cycle and calculate the ensemble (average) prediction at each hour.

Graphical Approach

The two-harmonic, generalized dimensionless model, $NEE^{*}_{\text{mod}}(t)$ was estimated for all 24 h of a diurnal cycle by using the spatiotemporally averaged (ensemble) parameter set (last row of Table 2), which incorporated four reference times (t_{ref} = 11–14 h) for both marshes. The estimated $NEE^{*}_{\text{mod}}(t)$ were then plotted with the corresponding hours of a day (Fig. 9). However, a user can plot similar graphs of $NEE^{*}_{\text{mod}}(t)$ using the site-specific set of parameters for different reference times (Table 2). The generalized model plot can be utilized by users to graphically obtain $NEE^{*}_{\text{mod}}(t)$ for all diurnal hours. The users should then multiply the estimated $NEE^{*}_{\text{mod}}(t)$ by a reference observation of NEE (NEE_{ref}) collected any time during 11 A.M. to 2 P.M. to predict the corresponding diurnal cycle of hourly NEE at any of the two marshes. Given that $NEE^{*}_{\text{mod}}(t)$ is dimensionless (i.e., unitless), the chosen units of NEE_{ref} will determine the units of NEE for all 24 h. Therefore, any user-defined units (e.g., µmol/m^2/s, gC/m^2/s, tonC/ha/day) can be chosen for NEE_{ref} to obtain the hourly NEE in the corresponding units.

Using the Final Model Equation

For users keen to using mathematical equations, the final form of the generalized two-harmonic model may be preferable to

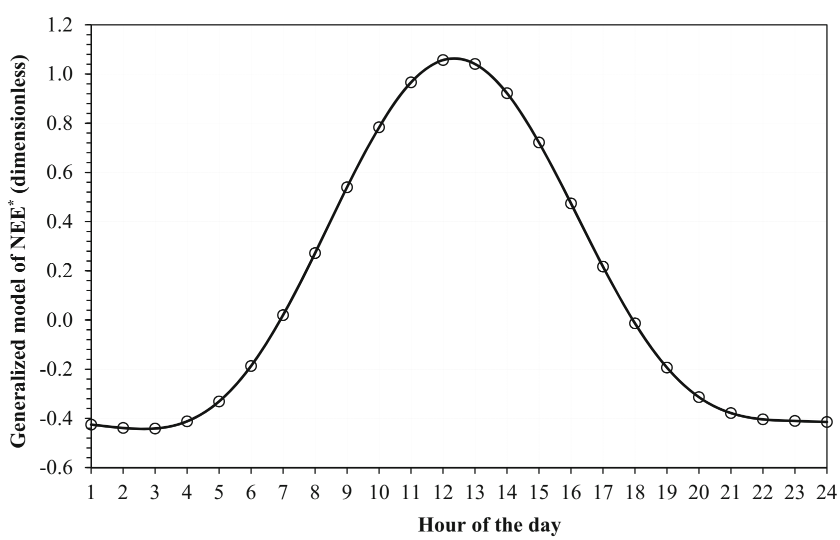


Fig. 9 Diurnal hours vs. the generalized NEE* model to graphically estimate NEE at any hour by multiplying NEE* with a single reference observation of NEE collected anytime during 11 A.M. to 2 P.M. The NEE* for each hour was calculated by using the generalized parameter set

the graphical approach. Using the spatiotemporally averaged parameter set (Table 2), Eq. 4 can be rearranged to obtain the final model of NEE as follows:

$$NEE(t) = NEE_{ref}\left[0.11{-}0.74\cos\left(\frac{\pi t}{12}\right){-}0.09\sin\left(\frac{\pi t}{12}\right) + 0.21\cos\left(\frac{\pi t}{6}\right) + 0.03\sin\left(\frac{\pi t}{6}\right)\right] \quad (5)$$

(5)

where t = any hour of the diurnal cycle (i.e., 1–24 h), and $\pi \approx$ 3.14159 rad or 180 degrees. However, subject to a user's discretion, the parameter values in Eq. 5 can be replaced by the site-specific parameter sets for different reference times (Table 2). For any Julian day of a year at any of the two marshes, the users simply need to provide a single reference observation (NEE_{ref}) collected anytime during 11 A.M. to 2 P.M. on the right-hand-side of Eq. 5 to predict NEE for all 24 h. The units of NEE will represent the chosen units of NEE_{ref} such as μmol/m^2/s, gC/m^2/s, tonC/ha/day, and so on.

Using the Attached Excel Spreadsheet Model

A user-friendly, macro-based Excel spreadsheet model named "Florida Everglades NEE Model" is presented to simulate the diurnal cycles of hourly NEE from the day- and site-specific reference observation (NEE_{ref}) at the two Everglades marshes (see Florida Everglades NEE Model 2017 to download the Excel model). The estimated ensemble parameter set along with the model application algorithm was coded in the Excel file using Visual Basic. A user can choose any of the parameter sets (site-specific values or spatiotemporally ensemble values) provided in Table 2 for estimation of the diurnal cycles. However, the generalized parameter set (last row in Table 2) was used in the Excel spreadsheet as a default. A "Readme" sheet is included therein to provide an overview and describe the necessary steps to run the model. An "Example" sheet is also provided to demonstrate the predictions of different diurnal cycles (randomly selected from both marshes) during 2009–10 using the corresponding reference observation (NEE_{ref}). Although all NEE were expressed in the units of μmol/m^2/s, any user-defined units (e.g., gC/m^2/s, tonC/ha/day) can be used to input NEE_{ref} to obtain the NEE for 24 h in the corresponding units. Upon enabling the "macros" in the Excel file, the users need to input the single reference observations (NEE_{ref}) measured during 11 A.M. to 2 P.M. along with the corresponding Julian days and years to estimate the respective diurnal cycles of hourly NEE with a single click on the "RUN".

Model Utility and Limitations

The presented model can be used to successfully estimate the fine-resolution (e.g., hourly) time-series of NEE from a limited number of observation for the Everglades freshwater wetlands. The increasing demand for wetland carbon accounting at longer time-scales and the existing gaps in the small-scale eddy-covariance observations of NEE, therefore, inherently indicate the utility of the harmonic model. Furthermore, a generalization of parameters across time and the two different marshes indicates an existence of similitude in ecosystem functions and overall response. The presented scaling-based method can, therefore, be potentially applied (upon re-calibrations) to estimate hourly NEE time-series at different wetlands and other ecosystem types (e.g., deciduous forests, evergreen needleleaf forests, mixed forests) using the available database (e.g., AmeriFlux, FluxNet). The harmonic model algorithm can also be applied to predict different ecohydrological and environmental variables (e.g., net radiation, latent heat flux, sensible heat flux, ground heat flux) that represent a cyclic pattern.

The scaling-based harmonic model cannot estimate a diurnal cycle of hourly NEE if no corresponding reference-time observation of negative NEE (i.e., uptake) is available for the day. Further, the model is not applicable for sites/time that do not show a periodic diurnal pattern in NEE. However, mathematical modeling in general is an abstraction of reality, and much details can inherently be lost in the abstraction methods — which contribute uncertainty in model predictions. The use of filtered and gap-filled data for the harmonic model calibrations (that required complete diurnal cycles) could introduce bias and uncertainty in parameter estimations and model predictions. The possible gap-filling bias was minimized by calibrating the model with only those diurnal cycles that had four or less consecutive hourly gaps. The estimated parameters did not show any notable seasonal trend or bias among the different Julian days, years, and sites (Fig. 4). Further, the successful model validations (site-specific, inter-site, and generalized levels) (Table 3, Table S1, Fig. 7, Fig. S2) with the larger sets of un-filled data indicated no discernable effects of data-filtering and gap-filling on model predictions. Nevertheless, if extreme noise (e.g., frequent spike) exists in a diurnal cycle perhaps due to large floods and/or nutrient pulses, the model may not perform as good as for the days that represent a more stable ecosystem response. However, the model parameters were insensitive to the large ranges of daily variation in PAR, temperature, water level, and nitrogen and phosphorous concentrations at the two Everglades marshes (Fig. 5, and Fig. S1 in Supplemental notes). The parameter robustness ultimately led to the successful predictions of different diurnal cycles of NEE, representing a considerable variation in the hydroclimatic and water quality drivers.

Conclusions

A generalized empirical model was developed to estimate the diurnal cycle of hourly NEE based on a corresponding single reference observation from the Florida Everglades freshwater wetlands. The model was evaluated with AmeriFlux data collected during 2008–13 from the Taylor Slough and Shark River Slough marshes, representing a short vs. long hydroperiod, respectively. The study validated the hypothesis that scaling of the diurnal cycles of NEE by the corresponding day- and site-specific single reference observations would lead to a general, dimensionless NEE cycle for all days and sites. The model involved five parameters, which exhibited spatiotemporal robustness by collapsing into narrow ranges among the different days and years across the two marshes. Estimated hourly NEE using the site-specific ensemble (averaged over all days) and the generalized (averaged over all days and sites) parameter sets indicated a good performance of the model (NSE = 0.66–0.89; RSR = 0.33–0.58). The empirical model only requires a single reference observation of negative NEE, collected anytime during 11 A.M. to 2 P.M., to predict the corresponding diurnal cycle. The model is represented in three standalone formats: (1) a simple final equation for direct calculation, (2) a single dimensionless cycle of hourly NEE for graphical estimation, and (3) a user-friendly Excel spreadsheet. Subject to the users' preferences, any of the three tools can be applied to estimate fine resolution (e.g., hourly) NEE time-series for the desired Julian days and years from the respective single reference observations. The harmonic model can, therefore, be applied as an empirical gap-filling method to estimate missing data in observed, continuous (e.g., hourly) time-series of NEE at the Everglades freshwater wetlands.

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