Evaluation and correction of noise related to physical processes in estimates of estuary metabolism

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Acknowledgments

Abstract

Reliable estimates of ecosystem metabolism depend on measures of dissolved oxygen (DO) flux that are dominated by biological processes. Long-term time series of DO measurements may include variation related to both biological and physical processses such that the use of observed data may be insufficient in many examples. Statistical modelling techniques that quantify variation in DO over time and tidal changes have the potential to isolate biological signals in DO variation to more accurately estimate metabolism. We used a simulation approach to create an observed DO time series as the summation of diel variation. A weighted regression method that estimates DO as a function of time and tidal height was used to normalize, or detide, the predicted DO signal. Comparisons of detided estimates with the known, simulated biological DO signal suggested the method accurately and precisely removed varation attributed to tidal advection. Extension of the method to four case studies provided a proof of concept illustrating the method could be useful for *in situe* data. We provide a detailed discussion on use of the method for improving certainty in evaluation of DO measurements from sites with strong tidal influences. Moreover, we propose that the method will greatly expand use of the open-water method for estimating ecosystem metaoblism given that the approach can provide robust estimates of DO values that are independent of tidal advection. This could facilitate the use of shorter deployment periods for water quality monitors or incomplete time series given that known biases related to water movement could be removed with weighted regression. {acro:DO}

Key words:

Introduction

{intro}

Ecosystem metabolism is broadly defined as the difference between primary production and aerobic respiration and provides a basis for evaluating trophic state (Kemp and Testa 2012, Needoba et al. 2012). Primary producers, such as phytoplankton, establish the means of energy transfer to upper trophic levels. Productive systems are characterized by more efficient transfer of organic matter between trophic levels, whereas less productive systems are sinks of organic matter that are supported by allochthonous sources of energy input. The balance between production and respiration is an integrated measure of metabolism that accounts for varying rates in processes that create and consume organic matter. Although metabolic rates vary naturally in different regions (Caffrey 2004), human activities and infrastructure development are contributing factors that increase rates of production (Diaz 2008). Inputs of limiting nutrients beyond background concentrations may decrease the resilience of an ecosystem such that higher rates of production are coupled with higher biological oxygen demand (Yin et al. 2004, Kemp et al. 2009). Cultural eutrophication is frequently linked to declines in water quality through lower levels of dissolved oxygen and increased frequency of noxious algal blooms. Reliables estimates of ecosystem metabolism are critical for measuring both background rates of production and potential impacts of human activities on ecosytem condition.

Ecosystem metabolism can be estimated using several techniques, each of which is appropriate under different conditions or assumptions. Bottle-based techniques rely on rate measurements from discrete water quality samples, whereas open-water techniques infer metabolic rates using *in situ* measurements from continuous monitoring data. Bottle-based techniques are useful for direct partitioning of metabolic contributions into discrete habitats, such as planktonic production rates during specific time periods (Kemp and Testa 2012). However, such measurements may be inappropriate for evaluating whole ecosystem metabolism if significant production occurs in habitats that are not sampled, such as benthic or seagrass production. As such, the open-water technique provides an integrative measure of metabolism by inferring process rates from *in situ*, continuous monitoring data. Originally proposed for use in streams (Odum 1956), the method has been used with varying success in lakes (Staehr et al. 2010, Coloso et al. 2011, Batt and Carpenter 2012) and estuaries (Caffrey 2004, Hopkinson and Smith 2005, Caffrey et al. 2013). The ability of the open-water method to accurately estimate metabolism depends on whether the assumptions for its use are met, which are often only implicity verified in practiced.

The open-water method uses the diel fluctuation of dissolved oxygen to infer rates of ecosytem metabolism, after correcting for losses or gains through air-water exchange (Kemp and Testa 2012). Daily integrated measurements of metabolism are based on the balance between daytime estimates of gross production and nighttime estimates of respiration extrapolated to a 24 hour period. The fundamental assumption of the open-water method is that measurements come from a water mass that has the same recent history (Needoba et al. 2012). Estimates of metabolism from a single location may be inaccurate if substantial variation in water column mixing occurs throughout the period of observation. As such, the original technique designed for use in streams requires the comparison of data from an upstream and downstream station (Odum 1956). Application of the method to systems without continuous flow, such as lakes or estuaries, have often assumed that a single sampling station provides sufficient data for estimating metabolism Staehr et al. (2010). While single stations may be valid under specific conditions, numerous studies have shown that the open-water method may be inappropriate given the effects of physical mixing (Ziegler and Benner 1998, Caffrey 2003, Coloso et al. 2011, Batt and Carpenter 2012, Nidzieko et al. 2014).

The open-water method has recently been applied to coastal and oceanic ecosystems with mixed success. An exhaustive analysis by Caffrey (2003) applied the method to estimate metabolim at 28 continuous monitoring stations at 14 US estuaries. Data from two of the reserves were used to evaluate the assumption of homogeneity of water masses measured by each sensor. Although significant differences were not observed for metabolism estimates between adjacent stations, the analysis was based on a comparison of means using conventional significance tests rather than a systematic comparison of time series. Moreover, a portion of metabolism estimates from all stations were negative for production during the day and positive for respiration during the night. These values were opposite in sign than expected since production increases oxygen during the day (i.e., positive effect on metabolism) and respiration consumes oxygen at night (i.e., negative effect on metabolism). These 'anamolous' values were attributed to violations in the assumption of water-column heterogeneity. Specifically, tidal variation could have caused sampling of different water masses by individual water quality sondes as water moved inland or seaward with changing tide.

The effects of tidal advection on estimates of ecosystem metabolism have been a point of concern in numerous studies (Ziegler and Benner 1998, Caffrey 2003, Collins et al. 2013, Howarth et al. 2014), although systematic estimates of its effects and methods for accounting for physical variation in dissolved oxygen (DO) measurements have been minimal. An exception is {acro:DO} presented by Nidzieko et al. (2014) through quantitative assessment of the effects of fortnightly tidal modulations on metabolism estimates. Using a control volume approach to measure fluxes into and out of a shallow tidal creek, significant biases in metabolism estimates were observed.

Net heterotrophy was observed during spring tides, whereas metabolism was balanced during neap tides. The timing of irradiance relative to the tidal cycle was a primary factor contributing to heterotrophy during summer months such that maximum tides occurred during the night, increasing total area for respiration. The results of the analysis, although specific to the study location, suggest that the effects of tidal advection on DO measurements are of primary concern when selecting locations and length of time for sonde deployment in estuaries. In many cases, the relative magnitude of these effects may be a significant source of bias without quantitative evaluation to determine the roles of biological and physical signals in DO measurements. Analytical techniques to evaluate and correct for tidal advection could improve certainty in metabolism estimates and also increase the use of data from shorter deployment periods if sources of bias are quantified and removed.

This article describes use of a novel method for quantifying and removing noise in estimates of ecosystem metabolim for estuaries. Specifically, we characterize the effects of tidal advection on DO observations to improve estimates of open-water metabolism with multi-year time series of high frequency (< one hour) water quality data. The focus of our analysis is the use of a weighted regression method previously developed for trend analysis of pollutant concentrations in streams and rivers (Hirsch et al. 2010). A weighted regression approach is applied to create dynamic predictions of DO as a function of time and tidal height change, which is then used to normalize, or detide, the DO signal. The analysis is presented in two steps. First, we apply a simulation approach to create time series of DO observations with known characteristics to evaluate ability of the weighted regression to predict the time series and remove the effects of tidal advection. Second, four case studies of multi-year time series are used to further explore use of the weighted regression approach to remove potential noise in DO signals from tidal advection. Comparisons of observed and detided DO values are compared, in addition to estimates of open-water metabolism before and after detiding of the DO time series. Overall, the analysis provides a means to improve certainty in conclusions from observed DO for evaluating the relative roles of biological and physical processes in estuarine systems. Applications of the weighted regression approach are expected to have wide-ranging implications for management and ecosystem monitoring by outlining strategies for obtaining water quality estimates with more accuracy.

Materials and Procedures

Weighted regression for modelling and detiding DO time series

The weighted regression model for detiding DO time series was adapted from the weighted regression on time, discharge, and season (WRTDS) method developed by Hirsch et al. (2010). The WRTDS method was developed to model pollutant concentration in streams and normalize predictions to changes in discharge. The functional form of our model is as follows: {acro:WRTI

$$DO_{obs} = \beta_0 + \beta_1 t + \beta_2 H \qquad (1)$$ {funform}

where observed DO is a linear function of decimal time t and astronomical tidal height H. Decimal time is a continuous variable for the day and time of each obervation with time as a proportion of the number of total observations added to each day. The beginning of each day was considered the nearest thirty minute observation (i.e., on the hour and half hour) at which sunrise was expected for a given location and time of year. Days were centered on the diel cycle rather than conventional times given that the objective was to develop a predictive model relevant for biological DO variation that follows solar and seasonal cycles. The functional form also differed from the original WRTDS method that included parameters to estimate variation of the response variable on a sinuisoidal period. DO variation was not modeled using this approach because rates of change may be abrupt following diurnal variation in irradiance or daily DO variation may be muted given the weather, as on cloudy days.

Weighted regression is implemented as a moving window that allows for estimation of DO throughout the time series by adapting to variation through time as a function of tide. Regression models are estimated sequentially for each observation in the time series using dynamic weight vectors that change with the center of the window. Weight vectors quantify the relevance of observations to the center of the window in respect to decimal time, hour of the day, and tidal height. Specifically, weights are assigned using a tri-cube weighting function (Hirsch et al. 2010):

$$w = \begin{cases} \left(1 - (d/h)^3\right)^3 & \text{if } |d| \leq h \\ 0 & \text{if } |d| > h \end{cases} \tag{2}$$

where the weight w of each observation is inversely proportional to the distance d from the center of the window such that observations more similar to the point of reference are given higher importance in the regression. Weights exceeding the maximum width of the window h are equal to zero. The tri-cube weighting function is similar to a normal distribution such that weights decrease gradually from the center until the maximum window width is reached. Observations that are half the distance from the center of the window to the maximum window width are weighted 1/3 less than values at the center. Regressions that use simpler windows (e.g., boxcar approach) are more sensitive to influential observations as they enter or leave the window, whereas the tri-cube function minimizes their effect through gradual weighting of observations (Hirsch et al. 2010). The weight vector for each observation is the product of three separate weight vectors for decimal time, hour, and tidal height. A low weight is given to an observation if any of the three weighting values were not similar to the center of the window since the final weight vector is the product of three weight vectors for each variable.

A nontrivial issue with weighted regression is the choice of window width for calculating weights. Excessively large or small window widths may respectively under- or over-fit the data. Additionally, optimal window widths may depend on the objective for using the model. The weighted regression approach can be used for both predicting DO and normalizing to remove the variance in the DO signal from tidal changes. Optimal window widths that minimize prediction error or fit to the observed data are typically smaller than the optimum window widths for normalizing the time series. Similarly, window widths that more effectively detide the DO signal may produce predictions for the observed data that are not optimal. Evaluations of the weighted regression method with simulated DO time series, described below, used different window widths to identify an approximate optimal window width for detiding the DO signal. As such, the ability of the models to predict observed DO was not a primary concern given that the optimal window width for detiding likely corresponds to a model that predicts DO as a function of tide rather than observed DO as a function of both tide and biological variation.

Detiding the DO signal using weighted regression

The primary objective of the analysis was to evaluate ability of the weighted regression method to detide a DO signal to obtain more accurate estimates of metabolism. Hirsch et al. (2010) developed the normalization approach for the WRTDS method using a two-dimensional interpolation grid that contains predicted values of pollutant concentrations across the time series and the range of stream discharge values observed in the study system (Hirsch et al. 2010). Normalized values for pollutant concentration are obtained by averaging the model predictions across the discharge values that are likely to occur on a given day to provide an estimate that is independent of flow variation.

Predicted values of DO concentration were normalized to remove variation from tidal height changes, although the approach herein differs slightly from Hirsch et al. (2010). Our approach uses weighted regression to isolate sources of variation in the observed DO signal that are related to unique effects of tidal height and biological process (Fig. 1). Two sets of values are predicted for the observed time series DO_{obs}, rather than creating an interpolation grid. The first set of values uses the tidal height of an observation and second set uses the mean tidal height across the time series, DO_{tid} and DO_{nrm} respectively. In other words, the first set of predictions represent DO as a function of time and tide, where the second set represents DO conditional on time and mean tidal height:

$$DO_{tid} = f(DO_{obs}|H, t) \tag{3}$$ {do_tid}

$$DO_{nrm} = f(DO_{obs}|\bar{H}, t) \tag{4}$$ {do_nrm}

Assessment

Simulation of DO time series

The ability of the weighted regression to detide the DO signal was evaluated first using a simulation approach. Observed DO time series were created to represent the sum of variation from biological processes and physical effects related to tidal advection:

$$DO_{obs} = DO_{bio} + DO_{adv} \quad (5)$$ {do_obs}

Biological DO signals are inherently noisy (Batt and Carpenter 2012) and can be further described as:

$$DO_{bio} = DO_{die} + DO_{unc} \quad (6)$$ {do_bio}

$$DO_{unc} = \epsilon_{obs} + \epsilon_{proc} \quad (7)$$ {do_unc}

where the biological DO signal is the sum of diel variation on a 24 hour scale plus uncertainty or noise. Total uncertainty in the biological DO signal is described as variation from observation and process uncertainty (Hilboron and Mangel 1997). Multiple time series at 30 minute observations over 30 days were created following eqs. (5) to (7) such that observed DO is generalized as the additive combination of four time series (Fig. 2):

$$DO_{obs} = DO_{adv} + DO_{die} + \epsilon_{obs} + \epsilon_{pro} \quad (8)$$ {do_obs_a

Time series were created by varying the relative magnitudes of each of the four components of observed DO to test the effectiveness of weighted regression under different scenarios. The effects of air-sea gas exchange were not considered in the simulation given that methods are available for *in situ* data to correct observed DO for diffusion (i.e., Thébault et al. 2008).

Each parameter of the simulated time series was created as follows. First, biological DO time series in eq. (6) were created by adding noise or variance to a diel component (Fig. 2). The diel component, DO_{die}, was estimated using a sine/cosine function (Cryer and Chan 2008):

$$DO_{die} = \alpha + \beta \cos\left(2\pi f t + \Phi\right) \qquad (9) \quad \{\texttt{do\_sin}\}$$

such that the mean DO α was 8, amplitude β was 1, f was 1/48 to repeat on a 24 hour period every 30 minutes, t was the time series vector and Φ was the x-axis origin set for an arbitrary sunrise at 630am. The diel signal was increasing during the day and decreasing during the night for each 24 hour period and ranged from 7 to 9 mg L^{-1}. Noise or uncertainty was added to the diel DO signal to simulate natural variation in DO throughout the time series (Fig. 2). Total uncertainty was the sum of observation and process uncertainty for $n = 1440$ (30 minutes by 30 days) observations (Hilboron and Mangel 1997), such that:

$$DO_{unc,n} = \epsilon_{obs,n} + \int_{t=1}^{n} \epsilon_{pro,t} \qquad (10) \quad \{\texttt{do\_unc\_n}$$

where observation and process uncertainty (ϵ_{obs}, ϵ_{pro}) were simulated as normally distributed random variables with mean zero and standard deviation varying from zero to an upper limit, described below. To induce auto-correlation, process uncertainty was estimated as the cumulative sum of n observations where the noise at time $t+1$ was equal to the noise at time t plus additional variation drawn from the normal distribution. The noise vector for process uncertainty was rescaled to constrain the variation within the bounds for standard deviation defined by the random variable. The total uncertainty, DO_{unc}, was added to the diel DO time series to create the biological DO time series (Fig. 2).

A tidal time series was simulated by adding sine waves (harmonics) with relevant solar and lunar periods (Foreman and Henry 1989). Each sine wave was created using eq. (9) by varying f for periods that approximated common tidal components, e.g., 1/25 for a 12.5 hour principal lunar semi-diurnal wave. The amplitude of each tidal component was set constant to one meter. The combined tidal series was the additive time series of all sine waves, scaled to 1 meter and centered at 4 meters. The tidal time series was added to the biological DO series to simulate DO changes with advection, DO_{adv} (Fig. 2). Conceptually, this vector represents the rate of change in DO as a function of horizontal water movement from tidal advection such that:

$$\frac{\delta DO_{adv}}{\delta t} = \frac{\delta DO}{\delta x} \cdot \frac{\delta x}{\delta t} \tag{11}$$ {deltdo}

$$\frac{\delta x}{\delta t} = k \cdot \frac{\delta H}{\delta t} \tag{12}$$ {deltx}

where the first derivative of the tidal time series, as change in height over time $\delta H / \delta t$, is multiplied by a constant k, to estimate horizontal tidal excursion over time, $\delta x / \delta t$. The horizontal excursion is assumed to be associated with a horizontal DO change, $\delta DO / \delta x$, such that the product of the two estimates the DO change at each time step from advection, DO_{adv}. In practice, the simulated tidal signal was used to estimate DO_{adv}:

$$DO_{adv} \propto H \tag{13}$$ {do_advp}

$$DO_{adv} = 2 \cdot a + a \cdot \frac{H - \min H}{\max H - \min H} \tag{14}$$ {do_adv}

where a is analogous to k in eq. (12) and is chosen as the transformation parameter to standardize change in DO from tidal height change to desired units. For example, $a = 1$ will convert H to a scale that simulates changes in DO from tidal advection that range from +/- 1 mg L^{-1}. The final time series for observed DO was the sum of biological DO and advection DO (Fig. 2).

Evaluation of weighted regression with simulated DO time series

Multiple time series were simulated by varying the conditions in eqs. (5) to (14). Specifically, the simulated data varied in the relative amount of noise in the measurement, relative amplitude of the diel DO component, degree of association of the tide with the DO signal, and tidal type as diurnal, semidiurnal, and mixed semidiurnal. Three levels were evaluated for each variable: relative noise as 0, 1, and 2 standard deviations for both process and observation uncertainty, amplitude of diel biological DO as 0, 1, and 2 mg L^{-1}, and DO change from tidal advection as 0, 1, and 2 mg L^{-1}. Three tidal categories were created from eq. (9) using a period of 24.82 hours (principal lunar) for diurnal, 12.42 hours (principal lunar semidiurnal) for semidiurnal, and adding both diurnal and semidiurnal series for mixed semidiurnal. A total of 243 time series were created based on 81 unique combinations of parameters for each tidal category (Fig. 3). Three window widths for each variable used to estimate the total weight vetor were evaluated (as half window widths): decimal time as 1, 3, and 8 days, time of day as 6, 12, and 24 hours, and tidal height as 0.25, 0.5, and 1 as a proportion of the observed value at the center of the window. In total, 27 window width combinations were evaluated for each of 243 simulated time series, producing results for 6561 weighted regressions.

The detided or normalized values for each regression were compared to the simulated data to evaluate the ability of weighted regression to reproduce the biological DO signals. Results were summarized using Pearson correlation coefficients and the root mean square error (RMSE) {acro:RMSE between the predicted and observed DO values and the detided and biological DO values.

Overall, the weighted regressions provided accurate results for the detided time series compared to the 'true' biological time series regardless of the simulation parameters (Table 1) or window widths (Table 2). Mean correlation for all time series and window widths between the detided and biological values was NA, with values ranging from -0.78 to 1.00. Mean error was 1.27, with values ranging from 0.00 to 2.47. Simulations with very poor performance (e.g., negative correlations) were those that had minimum widths for day windows and maximum widths for hour windows, or were those with the DO signal composed entirely of noise from observation uncertainty. Characteristics of DO time series that contributed to improved model performance were increasing amplitude of the diel DO component (DO_{die}) and increasing process uncertainty (e_{pro}), whereas increasing observation uncertainty contributed to decreasing performance (Table 1). Model performance was not related to magnitude of the tidal advection component (DO_{adv}), whereas models with diurnal tidal components had slightly decreased performance. Increasing widths for day and tidal proportion windows contributed to increasing model performance, whereas the opposite was true for increasing hour windows (Table 2).

A closer examination of the results for unique scenarios can provide additional insight into characteristics of observed DO that influence model results. In particular, the performance of the model depends entirely on the ability to predict variation in DO from tidal effects (DO_{tid}, Fig. 1) and the mean response of DO conditional given constant tidal height (DO_{mtd}, Fig. 1). Specific characteristics of the DO time series (e.g., relative magnitude of ϵ_{proc}, DO_{adv}, etc.) influence the ability of the model to predict unique sources of variation in observed DO. An extreme case is presented by time series that have no influence of tidal advection (i.e., $DO_{adv} = 0$) on the observed time series. **??** shows the model results from a simulated time series with no tidal component and the observed DO signal is composed only of a diel component

($DO_{bio} = 2$). Although the ‘correct’ results were obtained with large window widths, the model predicts increasingly periodic contributions of the tidal (DO_{tid}) and mean tidal component (DO_{mtd}) with decreasing window widths. These results can be explained by phase synchrony or asynchrony between the simulated tidal component and observed DO as the model fits the time series to a non-existent tidal advection component. As window width decreases, higher importance is given to observations within the window such that periods with high synchrony or asynchrony between observed DO and the tidal component will have a larger influence on the model parameters. Although application of the model to such a time series would be impractical, the results illustrate the importance of preliminary evaluations of the data and considerations for window widths. Time series with no obvious effect of tidal advection should use relatively large window widths because results from small window widths may be impractical.

Validation of weighted regression with case studies

The National Estuarine Research Reserve System (NERRS) is a federally-funded network {acro:NERR
of 28 protected estuaries established for long-term research, water-quality monitoring, education, and coastal stewardship (Wenner et al. 2004). Continuous water quality data have been collected at NERRS sites since 1994 through the System Wide Monitoring Program (SWMP). In addition {acro:SWMP
to providing a basis for trend evaluation, data from SWMP provides an unprecedented opportunity to evaluate variation in water quality parameters attributed to both biological and physical processes. Continuous SWMP data describe DO variation at sites with different characteristics, including wide ranges in tidal regime (Sanger et al. 2002) and rates of ecosystem production (Caffrey 2003).

Water quality from the SWMP database (CDMO 2014) were used to validate the weighted regression model beyond simulated time series. Continous monitoring data from January 1st to December 31st 2012 were obtained for four stations representing a range of geographic locations (Fig. 6 and Table 3). Each station was chosen specifically using measured correlations between DO and tidal changes, suggesting strong influences of physical processes as potential confounding factors in biological DO signals. The four sites included Joe Leary estuary station at Padilla Bay (Washington, 48.52°N 122.48°W), Middle Blackwater River station at Rookery Bay (Florida, 25.93°N 81.60°W), Dean Creek station at Sapelo Island (Georgia, 31.39°N 81.28°W), and Boca Rio station at Tijuana River (California, 32.56°N 117.13°W).

Estimates of ecosystem metabolism before and after detiding

The weighted regression method was applied to the time series for each station to obtain a detided DO estimate for estimating metabolism. A window width of twenty days was used as a median value between the extremes evaluated in the simulations. Unlike the simulated data, the true biological DO signal was unknown for the case studies. Accordingly, results were evaluated based on differences between the observed and detided DO time series, as well as correlations of DO and metabolism estimates with tidal height before and after application of the model. Astronomical tidal heights were predicted for each site using sonde depth data and harmonic regressions (`oce` package in R, Foreman and Henry 1989, RDCT 2014). We hypothesized that metabolism esimates using the detided signal would contain less ‘anomalous’ values than those from the observed DO time series, where ‘anomalous’ was defined as negative production estimates during the day and positive respiration estimates during the night. Although anomalies could be caused by processes other than tidal advection, e.g., abiotic dark oxygen production (Pamatmat 1997), we assume that physical processes are the dominant sources of these values.

Ecosystem metabolism was estimated using the open-water technique (Odum 1956) as described in Caffrey et al. (2013). The method is used to infer net ecosystem metabolism from DO time series using the mass balance equation:

$$\frac{\delta DO}{\delta t} = P - R + D \tag{15}$$

where the change in DO concentration (δDO, mmol O_2 m^{-3}) over time (δt, hours) is equal to photosynthetic rate (P, mmol O_2 m^{-3} hr^{-1}) minus respiration rate (R, mmol O_2 m^{-3} hr^{-1}) corrected for the rate of air-sea gas exchange at the interface (D, mmol O_2 m^{-3} hr^{-1}) (Caffrey et al. 2013). D is estimated as the difference between the DO saturation concentration and observed DO, multiplied by a volumetric reaeration coefficient, k_a (Thébault et al. 2008). The diffusion-corrected DO flux estimates were averaged during day and night for each 24 hour period in the time series, where flux is an hourly rate of DO change as the difference between observations at time t and $t + 1$. Areal respiration rates were assumed constant during the night and substracted from daily gross production estimates to yield net ecosystem metabolism (Table 3).

The effects of detiding the DO time series for each case study varied for DO observations and metabolism estimates (Table 4). Correlations of observed DO time series with predicted tidal height were highly significant, with all sites indicating positive relationships except Padilla Bay where tidal increases were associated with declines in DO concentration. Metabolism estimates using observed DO were compared with daily tidal ranges at each site since the estimates represent daily integrated values. Metabolism estimates from observed DO were only correlated for gross production at Elkhorn Slouth and net ecosystem metabolism for Rookery Bay (Table 4).

The detided DO time series had no significant correlations with tidal height change, whereas trends were unclear when evaluating correlations of daily tidal range with metabolism estimates based on the detided DO time series. For example, correlations with daily tidal range for metabolism estimated with detided time series were either unchanged (e.g., net metabolism for Rookery Bay), reduced (e.g., production for Padilla Bay), or increased (e.g., respiration for Rookery Bay) from those using observed DO. Instantaneous DO flux estimates (corrected for air-sea gas exchange) form the basis of metabolism estimates and were also evaluated for correlations to tidal changes before and after detiding the observed DO signals. Similar to DO, correlations of DO flux were substantially reduced although relationships were still significant (Table 4).

The effect of detiding DO time series varied for each case study (Table 5). The percent of daily integrated metabolism estimates that were anomalous (negative production, positive respiration) before detiding were higher for Elkhorn Slouth and Padilla Bay as compared ot Rookery Bay and Sapelo Island. The percent of anomalous metabolism values after detiding changed for each site, with increases for Elkhorn Slough and Padilla Bay, and decreases for Rookery Bay and Sapelo Island. Increases were largest for Elkhorn slough such that percent anomalous estimates for productiona and respiration increased by approximately 50%. Reductions were largest for Sapelo Island such that the percent anomalous values for production were decreased by approximately 50%. Metabolism estimates using detided DO also had decreased mean production and respiration (i.e., increasing trend towards more balanced metabolism) for Elkhorn Slough and Padilla Bay, whereas mean production and respiration estimates were generally unchanged for Rookery Bay and Sapelo Island. All case studies had less heterotrophic net metabolism estimates (i.e., less negative) after detiding, in addition to decreases in the standard error for all metabolism estimates.

An example from Sapelo Island further highlights the effects of weighted regression on metabolism estimates (Fig. 7). Tidal predictions for Sapelo Island indicated that the site is strongly semidiurnal with approximately two tidal peaks per 24 hour period. Tidal ffects on the observed DO time series were apparent such that semidiurnal variation is closely correlated to tidal height variation. Weighted regression was successful in removing the variation in the observed DO time series from changes in tidal height. The detided DO time series exhibited more consistent diel variation with photoperiod (i.e., one peak per 24 hours) as compared to the observed time series (i.e., two peaks per 24 hours). However, metabolism before and after detiding for the period of observation was similar, suggesting that detiding the DO signal does not have a large effect on mean daily integerated metabolism estimates.

Discussion

Comments and recommendations

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Figures

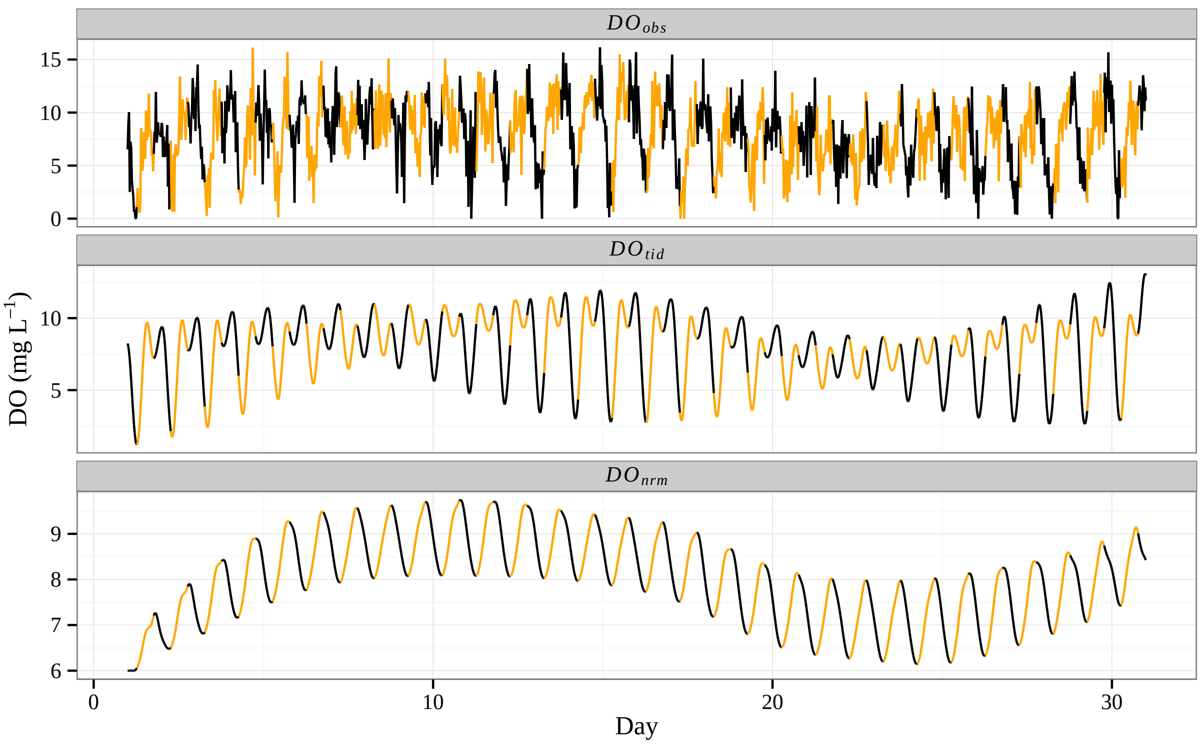

Fig. 1: Example of detiding a simulated DO time series. Simulated values are those in Fig. 2. Yellow indicates daylight periods. fig:do_dtd

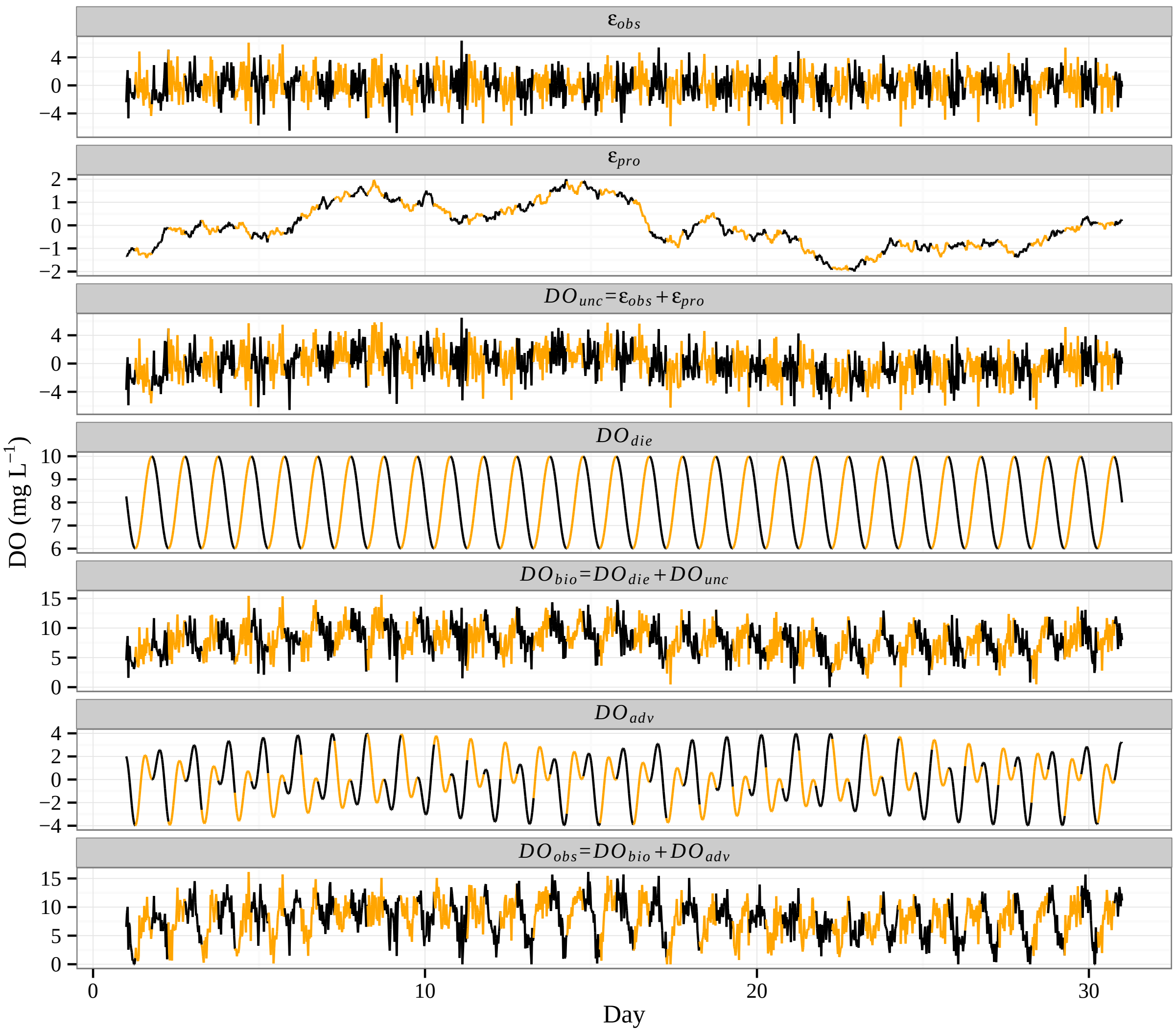

Fig. 2: Example of creating a simulated DO time series. Values were simulated every 30 minutes for 30 days. Yellow indicates daylight periods. fig:do_sim

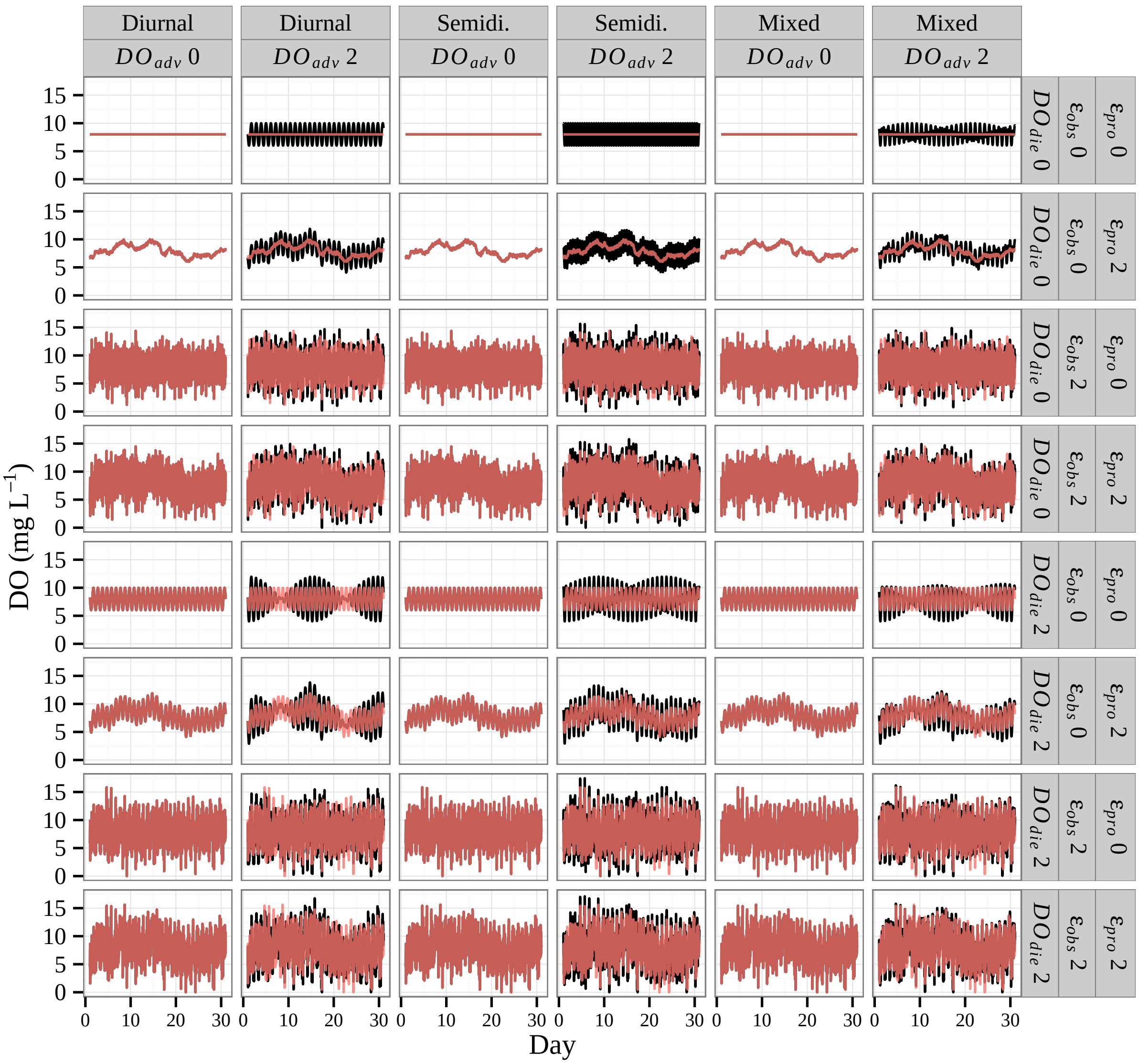

Fig. 3: Representative examples of simulated DO time series created by varying each of five parameters: tidal category (e.g., Mixed), strength of tidal association with DO signal using DO_{adv}, amount of process uncertainty ϵ_{pro}, amount of observation observation uncertainty ϵ_{obs}, and strength of diel DO component DO_{die}. Parameter values represent the extremes used in the simulation (i.e., minimum, maximum). Black lines are observed DO from eq. (8) and red lines are biological DO from eq. (6).fig:sim_ex

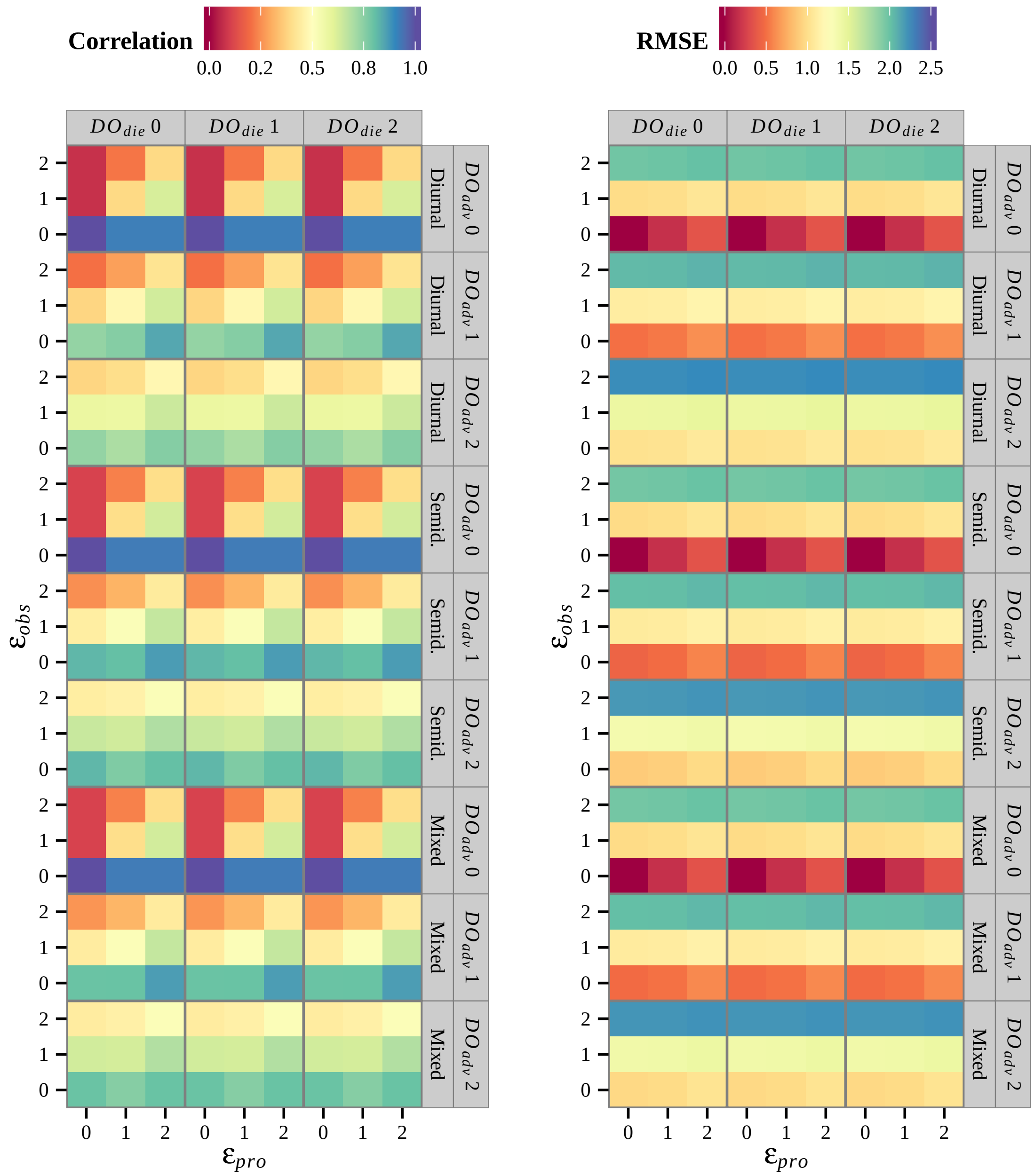

Fig. 4: Correlations and errors (RMSE) for detided DO time series, DO_{dtd}, from weighted regression with 'true' biological DO, DO_{bio}, for varying simulation parameters: tidal category (e.g., Mixed), strength of tidal association with DO signal DO_{adv}, amount of process uncertainty ϵ_{pro}, amount of observation observation uncertainty ϵ_{obs}, and strength of diel DO component DO_{die}. Each tile represents the correlation or error between detided and biological DO time series from results for a given combination of simulation parameters. Results are averaged for all window widths used to evaluate the regressions. fig:err_surf1

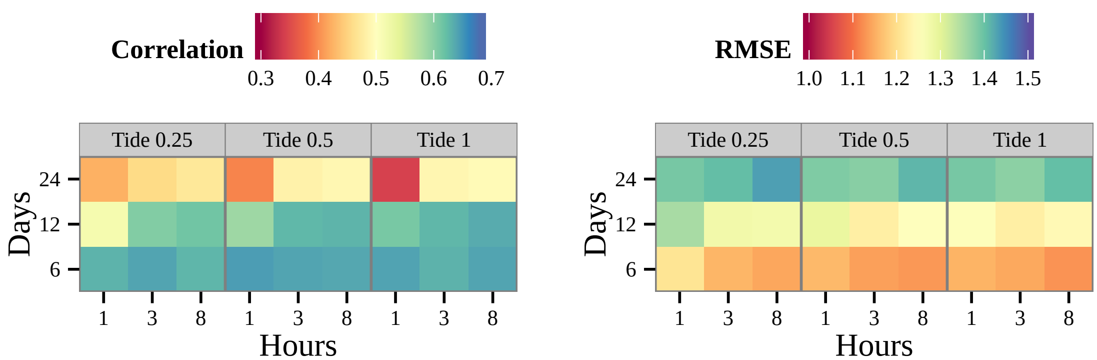

Fig. 5: Correlations and errors (RMSE) for detided DO time series, DO_{dtd}, from weighted regression with 'true' biological DO, DO_{bio}, for varying half window widths: days, hour of day, and proportion of tidal range. Each tile represents the correlation or error between detided and biological DO time series from results for a given combination of window widths. Results are averaged for all simulation parameters used to evaluate the regressions. fig:err_surf2

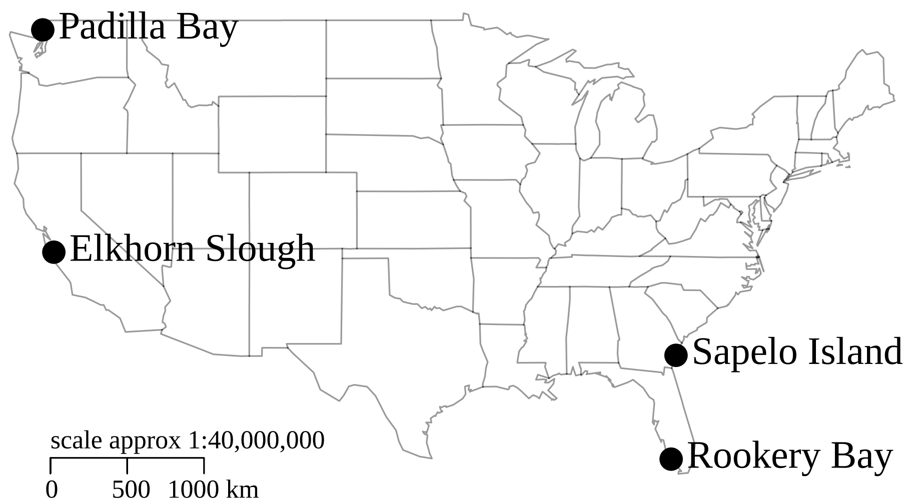

Fig. 6: Locations of NERRS sites used as case studies to evaluate of weighted regression. Individual stations at each reserve are PDBJE (Joe Leary Estuary at Padilla Bay), RKBMB (Middle Blackwater River at Rookery Bay), SAPDC (Dean Creek at Sapelo Island), and TJRBR (Boca Rio at Tijuana River). fig:case_map

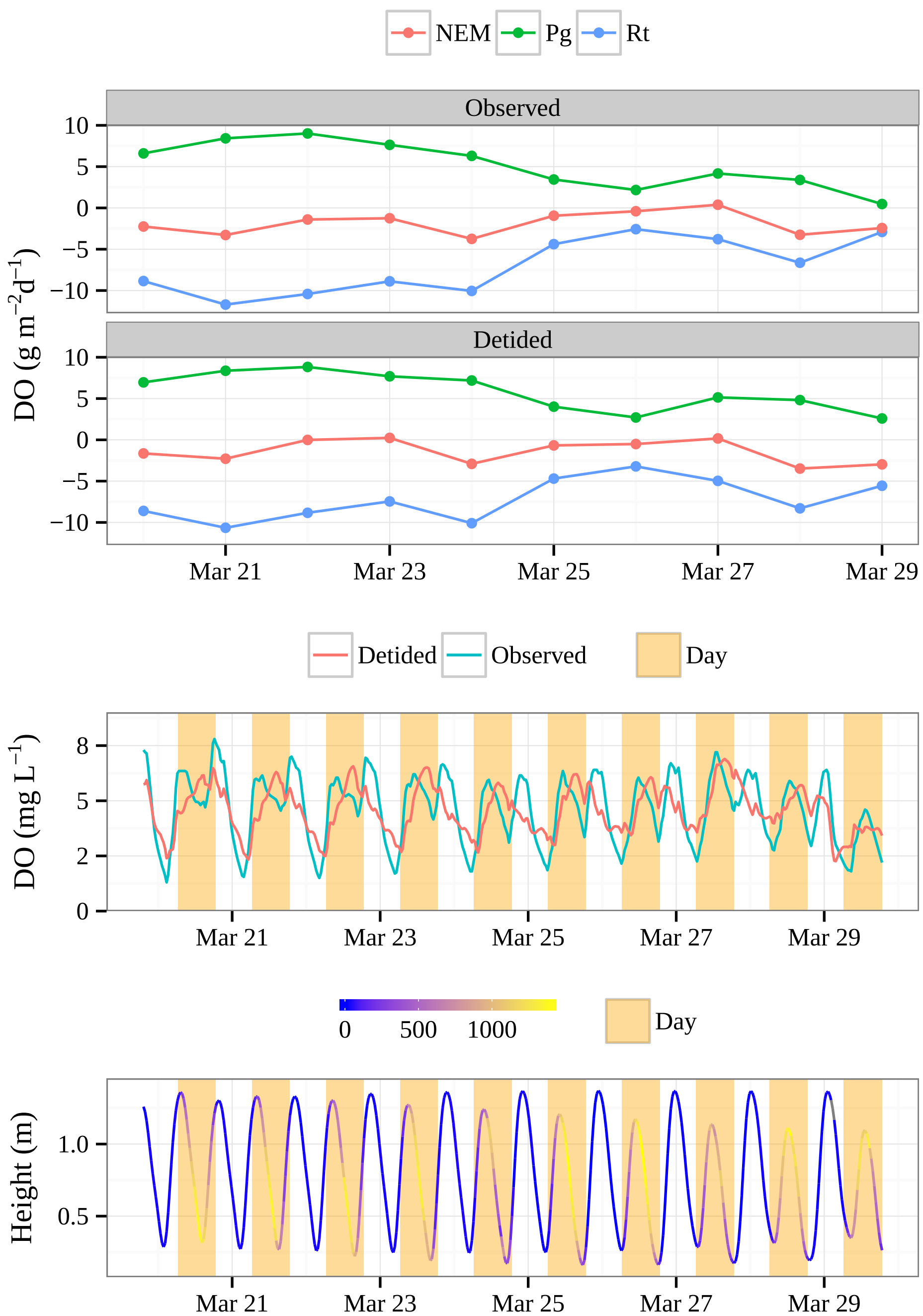

Fig. 7: Example of metabolism and DO time series before (observed) and after (detided) weighted regression. Results are for a ten day period in March for the Sapelo Island station using a weighted regression with a window of thirty days and tidal height proportion of one. fig:case_ex1

Tables

Table 1: Summary (range, mean, percentiles) of correlations and error estimates comparing detided and biological DO time series for different simulation parameters (tidal category, DO_{die}, DO_{adv}, ϵ_{pro}, ϵ_{obs}). Values represent a combination of results from multiple simulations with the parameter value held constant for each row (e.g., row one is a summary of all simulations for which the tidal category was diurnal). tab:dtd_perf1

Parameter	**Correlation**					**RMSE**				
	Min	25th	Mean	75th	Max	Min	25th	Mean	75th	Max
Tidal category										
Diurnal	-0.78	0.35	0.54	0.80	1.00	0.00	0.86	1.29	1.99	2.39
Semidiurnal	-0.28	0.37	0.58	0.84	1.00	0.00	0.73	1.25	1.97	2.40
Mixed Semidiurnal	-0.39	0.37	0.57	0.83	1.00	0.00	0.78	1.27	1.97	2.47
$\boldsymbol{DO_{die}}$										
0	0.00	0.21	0.52	0.92	1.00	0.00	0.26	1.05	1.96	2.05
1	-0.78	0.36	0.55	0.74	1.00	0.12	0.68	1.23	2.00	2.13
2	-0.78	0.48	0.62	0.81	1.00	0.25	1.13	1.53	2.08	2.47
$\boldsymbol{DO_{adv}}$										
0	-0.78	0.36	0.56	0.82	1.00	0.00	0.78	1.27	1.98	2.47
1	-0.78	0.36	0.56	0.82	1.00	0.00	0.78	1.27	1.98	2.47
2	-0.78	0.36	0.56	0.82	1.00	0.00	0.78	1.27	1.98	2.47
$\boldsymbol{\epsilon_{pro}}$										
0	-0.78	0.14	0.50	0.83	1.00	0.00	0.74	1.23	1.96	2.45
1	0.14	0.35	0.55	0.81	0.99	0.07	0.76	1.26	1.98	2.45
2	0.33	0.47	0.65	0.82	0.99	0.15	0.82	1.32	2.00	2.47
$\boldsymbol{\epsilon_{obs}}$										
0	-0.78	0.80	0.84	0.97	1.00	0.00	0.26	0.57	0.78	1.57
1	-0.07	0.39	0.51	0.67	0.84	0.96	1.01	1.18	1.25	1.82
2	0.00	0.22	0.34	0.44	0.63	1.93	1.98	2.07	2.11	2.47

Table 2: Summary (range, mean, percentiles) of correlations and error estimates comparing detided and biological DO time series for simulations using different half window widths in the weighted regressions (days, hours, and proportion of tidal range). Values represent a combination of results from multiple simulations with the window value held constant for each row (e.g., row one is a summary of all simulations for which the half window width was one day). tab:dtd_perf2

Window	**Correlation**					**RMSE**				
	Min	25^{th}	Mean	75^{th}	Max	Min	25^{th}	Mean	75^{th}	Max
Days										
1	-0.78	0.30	0.53	0.77	1.00	0.00	0.95	1.29	1.96	2.40
3	0.00	0.39	0.58	0.83	1.00	0.00	0.75	1.26	1.98	2.43
8	0.03	0.36	0.58	0.85	1.00	0.00	0.78	1.27	1.99	2.47
Hours										
6	0.00	0.41	0.64	0.90	1.00	0.00	0.53	1.15	1.97	2.21
12	0.04	0.41	0.61	0.85	1.00	0.00	0.87	1.27	1.98	2.33
24	-0.78	0.24	0.45	0.60	1.00	0.00	0.98	1.40	1.98	2.47
Tide										
0.25	0.03	0.35	0.55	0.81	1.00	0.00	0.81	1.29	1.99	2.47
0.5	-0.10	0.37	0.57	0.82	1.00	0.00	0.78	1.26	1.97	2.40
1	-0.78	0.36	0.57	0.82	1.00	0.00	0.76	1.26	1.97	2.40

Table 3: Summary statistics of tidal component amplitudes (m), DO (mg L^{-1}), and metabolism estimates (gross production, respiration, and net ecosystem metabolism as g m^{-2} d^{-1}) for each case study. Tidal components are principal lunar semidiurnal (O1, frequency 25.82 hours), solar diurnal (P1, 24.07 hours), lunar semidiurnal (M2, 12.42 hours), and solar semidiurnal (S2, 12 hours), estimated from harmonic regressions of tidal height (`oce` package in R, Foreman and Henry 1989, RDCT 2014). DO range and mean are grand means of daily estimates for the entire period of record (30 minute observations) for each site. Metabolism estimates are means of daily integrated values. tab:case_att

Site	**Tidal amplitude**				**DO**		**Metabolism**[a]		
	O1	P1	M2	S2	Range	Mean	Pg	Rt	NEM
ELKVM	0.24	0.12	0.48	0.13	6.79	7.86	5.42	-8.58	-3.16
PDBBY	0.46	0.23	0.63	0.15	7.53	8.97	8.03	-8.59	-0.56
RKBMB	0.13	0.04	0.36	0.10	5.47	4.53	2.46	-3.24	-0.78
SAPDC	0.10	0.02	0.54	0.07	7.98	5.01	4.46	-6.37	-1.90

[a]Pg: gross production, Rt: respiration, NEM: net ecosystem metabolism

Table 4: Correlations of tidal changes at each site with continuous DO observations, instantaneous DO flux, and metabolism estimates (gross production, respiration, and net metabolism) before (observed) and after detiding with weighted regression. DO values are correlated with predicted tidal height at each observation, DO flux values are correlated with tidal change between observations, and metabolism estimates are correlated with mean tidal change between observations during day, night, or total, day periods for production, respiration, and net metabolism respectively. Total day periods were defined as the approximate 24 hours between sunrises for two calendar days, where day was the time from sunrise to sunset and night was the following time from sunset to sunrise. Results are for weighted regressions using a window of thirty days and tidal height proportion of one. tab:cor_res

Site	DO	Pg[a]	Rt	NEM
ELKVM				
Observed	0.48***	0.43***	0.72***	0.02
Detided	-0.04***	-0.13*	-0.27***	0.03
PDBBY				
Observed	-0.45***	-0.14*	-0.27***	-0.15*
Detided	0.05***	0.43***	0.38***	-0.18**
RKBMB				
Observed	0.28***	0.35***	0.37***	0.14*
Detided	-0.02**	-0.36***	-0.45***	0.05
SAPDC				
Observed	0.48***	0.46***	0.62***	0.17**
Detided	-0.02*	-0.01	0.17**	-0.09

*$p < 0.05$; **$p < 0.01$; ***$p < 0.001$
[a]Pg: gross production, Rt: respiration, NEM: net ecosystem metabolism

Table 5: Summary of metabolism estimates (gross production, respiration, and net metabolism) for case studies using DO time series before (observed) and after (detided) application of weighted regression. Means and standard errors are based on daily integrated metabolism estimates. Anomalous values are the proportion of metabolism estimates that were negative for gross production and positive for respiration. Results are for weighted regressions with a window of thirty days and tidal height proportion of one. tab:case_res

Site	**Pg**[a]			**Rt**			**NEM**	
	Mean	Std. Err.	Anom	Mean	Std. Err.	Anom	Mean	Std. Err.
ELKVM								
Observed	5.42	0.70	0.28	-8.58	0.78	0.23	-3.16	0.40
Detided	2.81	0.19	0.13	-2.83	0.21	0.15	-0.02	0.05
PDBBY								
Observed	8.03	0.70	0.20	-8.59	0.78	0.16	-0.56	0.57
Detided	7.82	0.50	0.05	-7.82	0.50	0.06	0.00	0.11
RKBMB								
Observed	2.46	0.14	0.14	-3.24	0.16	0.10	-0.78	0.09
Detided	2.61	0.08	0.00	-3.21	0.08	0.00	-0.59	0.04
SAPDC								
Observed	4.46	0.25	0.17	-6.37	0.27	0.11	-1.90	0.15
Detided	4.37	0.10	0.01	-5.54	0.11	0.00	-1.18	0.05

[a]Pg: gross production, Rt: respiration, NEM: net ecosystem metabolism