Improving estimates of ecosystem metabolism by reducing effects of tidal advection on dissolved oxygen time series

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4 Acknowledgments

- 5 We acknowledge the significant efforts of research staff and field crews from the System
- 6 Wide Monitoring Program of the National Estuarine Research Reserve System for providing
- access to high quality data sets. We thank Dr. Jane Caffrey for reviewing a manuscript draft and
- previous work on applications of the open-water method to estuarine monitoring data. This study
- 9 was funded by the US Environmental Protection Agency, but the contents are solely the views of
- the authors. Use of trade names does not constitute endorsement by the US government.

Abstract

In aquatic ecosystems, time series of dissolved oxygen (DO) have been used to compute estimates of integrated ecosystem metabolism. Central to this open water or "Odum" method is the assumption that the dissolved oxygen time series is a Lagrangian specification of the flow field. However, most DO time series are collected at fixed locations, such that the method must assume changes in dissolved oxygen principally reflect ecosystem metabolism and that effects due to advection or mixing can be neglected. A statistical model using weighted regression was 17 applied to separate variability in DO associated with metabolism from tidal variation or other advection in estuaries, thereby helping to partially relax this assumption and improve estimates of ecosystem metabolism. The method was developed and tested using a simulated DO time series with known biological and physical components, and then applied to one year of continuous 21 monitoring data from four water quality stations within the National Estuarine Research Reserve System. Overall, the approach is a useful way to reduce variability in estimates of ecosystem 23 metabolism caused by advection, particularly when the magnitude of tidal influence is high and correlations between tidal change and solar cycling are low. By reducing the effects of physical 25 transport on metabolism estimates, there may be increased potential to empirically relate metabolic rates to causal factors on times scales of several days to several weeks. Estimates of 27 variability associated with physical advection may also be more interpretable, since convolution of physical and biological effects can be reduced.

Introduction

Ecosystem metabolism describes the balance between production and respiration 31 processes that create and consume organic matter (Kemp and Testa 2012, Needoba et al. 2012). Light exposure experiments of water samples collected at discrete locations and times have traditionally been used to measure metabolic activity. Although highly controlled and precise, bottle-based methods are labor-intensive and not scalable to describe entire ecosystem rates. Bottle-based methods may also only reliably estimate production and respiration associated with planktonic processes, whereas significant contributions of ecosystem production can arise from other habitats, such as the benthos or seagrass patches. By contrast, open-water techniques have been increasingly used to estimate whole system metabolism given the availability of long-term, continuous time series of dissolved oxygen (Odum 1956, D'Avanzo et al. 1996). Daily integrated measurements of metabolism represent the balance between daytime production and nighttime respiration attributed to all ecosystem components. Open-water estimates also provide a basis for tracking ecosystem change over time and are more practical for capturing events or evaluating trends as compared to bottle-based approaches. Although metabolic rates vary naturally at different spatial and temporal scales (Ziegler and Benner 1998, Caffrey 2004, Russell and Montagna 2007), anthropogenic nutrient sources are often contributing factors that increase rates of production (Nixon 1995, NRC 2000). Reliables estimates of whole ecosystem metabolism are critical for measuring both background rates of production and potential impacts of human activities on ecosytem condition. The ability to accurately estimate whole system metabolism using the open-water method

depends on the degree to which assumptions of the theory are met (Staehr et al. 2010, Kemp and

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Testa 2012). The fundamental assumption is that the time series of dissolved oxygen (DO)
   represents a Lagrangian specification of the flow field that describes the same water mass over
   time (Needoba et al. 2012). The Lagrangian specification assumes that the time series
   characterizes individual fluid parcels regardless of location, as in a parcel of water moving with
   the tide. In reality, most DO time series are collected at fixed locations such as a mooring or dock,
   which is characteristized by an Eulerian specification of the flow field. Time series at fixed
   locations may characterize water masses with different metabolic histories if water particles are
   transported by physical advection. A Lagrangian flow field is often assumed, such that estimates
   of metabolism may be inaccurate if substantial variation in water column mixing occurs
   throughout the period of observation (Kemp and Boynton 1980, Russell and Montagna 2007).
   Given this critical challenge, the open-water method has been used with varying success in
   estuaries influenced by tidal mixing (Caffrey 2004, Russell and Montagna 2007, Caffrey et al.
   2014). In contrast, the method has been more successfully applied to water quality time series in
   lakes, although stratification may limit estimates to specific vertical layers (Staehr et al. 2010,
   Coloso et al. 2011, Batt and Carpenter 2012). Appropriate placement of monitoring sondes,
   sampling frequency and duration, and reliability of data from single stations have been relevant
   issues in applying the open-water method to systems influenced by physical mixing (Russell and
   Montagna 2007, Staehr et al. 2010). Individual sampling stations near bay inlets or along major
   tidal axes may produce DO time series that fail to meet the assumptions of the open-water method.
           Although numerous studies have shown that application of the open-water method to lakes
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   or estuaries may be problematic (Ziegler and Benner 1998, Caffrey 2003, Coloso et al. 2011, Batt
   and Carpenter 2012, Nidzieko et al. 2014), very few quantitative approaches have been developed
   to address potential bias or noise in DO signals from physical advection. For example, an
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extensive analysis by Caffrey (2003) applied the open-water method to estimate metabolism at 28 continuous monitoring stations at 14 US estuaries. A significant portion of the production and respiration estimates were negative (3 - 69% depending on site), suggesting advection of water masses was a likely factor influencing the DO time series. These 'anomalous' values are typically omitted from the analysis (Caffrey 2003, Collins et al. 2013), which may upwardly bias estimates of metabolism (Caffrey et al. 2014). Further, Nidzieko et al. (2014) evaluated the effects of tidal advection on metabolism estimates in a mesotidal estuary. Estimates from a single location were 81 strongly correlated with the spring-neap cycle such that net heterotrophy was more common during spring tides, whereas metabolism was generally balanced during neap tides. A control-volume approach was used by impounding a section of the upper estuary to understand how physical processes contribute to biological variability. Although useful as an in situ, site-specific approach, more accessible statistical methods specific to time series are needed given the increasing availability of continuous monitoring data. For example, Batt and Carpenter (2012) explored the use of a Kalman filter (Harvey 1989) to remove process and observation uncertainty from DO time series in lakes. Similar approaches have not been developed for estuaries, particularly those that address potential effects of tidal advection.

This article describes the development and application of a method for improving estimates of ecosytem metabolism computed from DO time series. Specifically, the apparent effects of tidal advection on DO observations are removed to improve the fidelity of open-water metabolism estimates derived from continuous water quality data. We used a weighted regression approach originally developed to resolve trends in pollutant concentrations in streams and rivers (Hirsch et al. 2010). The weighted regression approach creates dynamic predictions of DO as a function of time and tidal height change, which are then used to filter, or detide, the DO signal.

The model is based on the recognition that daily fluctuations in DO are caused by metabolism associated with the solar cycle, whereas other fluctuations in estuaries are likely associated with water level changes that generally exhibit pregression relative to the solar cycle. The weighted regression model was applied, rather than methods commonly used for detiding in physical oceanography, to allow for the complex and dynamic patterns of DO changes relative to 102 advection. First, we used simulated DO time series with known characteristics to evaluate ability 103 of the weighted regression to remove the simulated effects of a tidally-advected DO gradient. 104 Second, the simulation results informed the application of the method to four case studies chosen 105 from the National Estuarine Research Reserve System (NERRS, Wenner et al. 2004). In all 106 examples, tidal height is used as a proxy for lateral water movements that may influence DO 107 observations. In the absence of quantitative data describing lateral DO variation (e.g., 108 contemporaneous stations along a tidal axis), we assume tidal height is an appropriate 109 characterization of lateral variation. Accordingly, 'tidal variation' or 'changes in tidal height' are 110 used throughout in reference to assumed lateral DO gradients that are carried past monitoring 111 sensors by tidal currents.

Materials and Procedures

Weighted regression for modelling and filtering DO time series

For this study, we adapted a weighted regression model to filter DO time series for apparent tidal effects. This model relied heavily on concepts used to develop the weighted regression on time, discharge, and season (WRTDS) method for estimating pollutant

concentrations in streams and rivers (Hirsch et al. 2010). The functional form of the model is:

$$DO_{obs} = \beta_0 + \beta_1 t + \beta_2 H \tag{1}$$

where DO_{obs} is a linear function of time t and tidal height H. Time is a continuous variable for the day and time of each observation as a proportion of the number of total observations added to each day. The beginning of each day was defined as the nearest thirty minute observation to 121 sunrise for the location. Our model differed from the original WRTDS method that included parameters to estimate variation of the response variable on a sinuisoidal period. DO variation 123 was not modeled using this approach to avoid constraining parameter estimates by periodic, diel 124 components. Additionally, a more desirable parameter for modelling the effects of tidal advection 125 on observed DO would be a direct measure of horizontal water movement, rather than tidal height 126 as used above. Although this approach would more accurately describe the theoretical foundation 127 of the mechanism, tidal height is an appropriate proxy given that the model is empirical and only 128 requires a variable that is correlated with the true measure of interest. We suspect that differences 129 in results using a measure of lateral advection as compared to tidal height as a predictor would be 130 minimal. 131

Weighted regression was implemented as a moving window that allowed for estimation of
DO throughout the time series by adapting to variation through time as a function of tide.

Regression models were estimated sequentially for each observation in the time series using
dynamic weight vectors that change with the center of the window. Weight vectors quantified the
relevance of observations to the center of the window in respect to time, hour of the day, and tidal
height. Specifically, weights were assigned to each variable using a tri-cube weighting function

138 (Tukey 1977, Hirsch et al. 2010):

$$w = \begin{cases} \left(1 - (d/h)^3\right)^3 & \text{if } |d| \le h\\ 0 & \text{if } |d| > h \end{cases}$$
 (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. Observations that exceed the maximum width of the window h are 141 assigned a weight of zero. The tri-cube weighting function is similar to a Gaussian distribution 142 such that weights are decreasing gradually from the center until the maximum window width is 143 reached. 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 145 minimizes their effect through gradual weighting of observations from the center (Hirsch et al. 146 2010). The final weight vector for each observation is the product of three separate weight vectors 147 for time (day), hour, and tidal height. Windows for time and hour are used to weight observations 148 based on distance (time) from the center of the window. The window for tidal height is used to 149 weight observations based on the difference from the center as a proportion of the total tidal 150 height range. For example, a half-window width of 0.5 means that observations are weighted 151 proportionately within +/- 50% the total range referenced to the tidal height in the center of the 152 window. A low weight is given to an observation if any of the three weighting values were not 153 similar to the center of the window since the final weight vector is the product of three weight 154 vectors for each variable (see the link in the multimedia section for graphical display of different 155 weights).

The choice of window widths for weight vectors strongly affects the model results. 157 Excessively large or small window widths may respectively under- or over-fit the observed data. Accordingly, appropriate window widths depend on the objective for using the model. The weighted regression approach can be used for both predicting observed DO and filtering the observed time series to remove the variance that coincided with the tidal cycle. Window widths 161 that minimize prediction error or fit to the observed data are typically smaller than widths that 162 would be used for filtering tidal effects. Similarly, window widths that more effectively filter the 163 DO signal may produce imprecise predictions for the observed data. Evaluations of the weighted 164 regression method with simulated DO time series, described below, used multiple window widths 165 to evaluate the ability of the model to filter the DO signal. The ability to predict observed DO was 166 not a primary objective such that the window widths were evaluated primarily based on the ability 167 to remove tidal variation from the DO time series. 168

The approach to filter physical advection from the observed DO time series differs slightly
from methods in Hirsch et al. (2010). The previous approach used a two-dimensional grid
predicted for stream pollutant concentrations across the time series and the range of discharge
values observed in the study system (Hirsch et al. 2010). Normalized or discharge-independent
values for pollutant concentration were obtained by averaging grid predictions across the
discharge values that were likely to occur on a given day. Rather than creating a two-dimensional
grid of DO related to time and tidal height change, the normalized time series herein were the
model predictions conditional on time and constant tidal height set to the mean:

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

such that the normalized time series represents DO variation related to biological processes. The
term 'filter' is used in reference to the removal of a specific variance component from the time
series, while maintaining the structure of the biological component. Although the approach shares
similarities with common filtering techniques, a distinction is noted such that weighted regression
has a specific purpose rather than the more generic objectives of common filters (e.g., moving
window averages or local smoothers, Shumway and Stoffer 2011).

33 Assessment

Simulation of DO time series

To test the ability of the weighted regression to filter the DO signal for apparent tide effects, multiple time series with known characteristics were simulated and filtered. A simulation approach was used prior to application with real data given that the true biological signal can be created as a known component for comparison with the filtered results from weighted regression. The following describes the theoretical basis for developing the simulated time series. Observed DO time series (DO_{obs}) were simulated as the sum of variation from biological processes (DO_{bio}) and physical effects related to tidal advection (DO_{adv}):

$$DO_{obs} = DO_{bio} + DO_{adv} (4)$$

Each component of DO_{obs} was simulated separately. The biological DO signal (DO_{bio}) was the sum of diel variation (DO_{die}) plus uncertainty or noise (DO_{unc}):

$$DO_{bio} = DO_{die} + DO_{unc} (5)$$

$$DO_{unc} = \epsilon_{obs} + \epsilon_{proc} \tag{6}$$

Biological DO signals are inherently noisy (Batt and Carpenter 2012) such that uncertainty in the biological DO signal was described as variation from observation and process uncertainty (ϵ_{obs} and ϵ_{pro} , Hilborn and Mangel 1997). Observation uncertainty is variation related to imprecision in 196 sampling processes or methods, whereas process uncertainty is caused by unknown parameters 197 that contribute to variance in a time-dependent fashion. Multiple time series at 30 minute time 198 steps over 30 days were created by varying the relative magnitudes of each of the components of 199 observed DO in eqs. (4) to (6) to test the effectiveness of weighted regression under different 200 scenarios. Accordingly, observed DO was generalized as the additive combination of four 201 separate time series (Fig. 1): 202

$$DO_{obs} = DO_{adv} + DO_{die} + \epsilon_{obs} + \epsilon_{pro} \tag{7}$$

Each component of the simulated time series was created as follows. First, the diel component, DO_{die} , was estimated (Cryer and Chan 2008):

$$DO_{die} = \alpha + \beta \cos(2\pi f t + \Phi) \tag{8}$$

such that the mean DO (α) was 8, amplitude (β) was 1, f was 1/48 to represent 30 minute intervals, t was the time series vector and Φ was the x-axis origin set for an arbitrary sunrise at 630. 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. Uncertainty was added to the diel DO signal as the

sum of observation and process uncertainty:

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$$DO_{unc,n} = \epsilon_{obs,n} + \int_{t=1}^{n} \epsilon_{pro,t}$$
 (9)

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. Process uncertainty was estimated as a serially correlated variable using the cumulative sum of n observations plus random variation added at each time step for t=1,...,n. The total uncertainty, DO_{unc} , was added to the diel DO time series to create the biological DO time series (eq. (5) and Fig. 1).

A semidiurnal tidal series was simulated with a period of 12.5 hours to represent the principal lunar component (Foreman and Henry 1989). The amplitude was set to 1 meter and centered at 4 meters. The tidal time series simulated DO changes with advection, DO_{adv} (eq. (7) and Fig. 1). Conceptually, this vector represents the rate of change in DO as a function of horizontal water movement from tidal advection such that:

$$\frac{\delta DO_{adv}}{\delta t} = \frac{\delta DO}{\delta x} \cdot \frac{\delta x}{\delta t} \tag{10}$$

$$\frac{\delta x}{\delta t} = k \cdot \frac{\delta H}{\delta t} \tag{11}$$

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} :

$$DO_{adv} \propto H$$
 (12)

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$$DO_{adv} = 2 \cdot a + a \cdot \frac{H - \min H}{\max H - \min H}$$
(13)

where a is analogous to k in eq. (11) 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 (eq. (4) and Fig. 1).

Evaluation of weighted regression with simulated DO time series

Multiple time series were simulated by varying the conditions in eq. (7) (Fig. 2) to 233 evaluate weighted regression under difference conditions. Specifically, the simulated data varied in the relative amount of noise in the measurement (e_{pro}, e_{obs}) , relative amplitude of the diel DO 235 component (DO_{die}) , and degree of association of the tide with the DO signal (DO_{adv}) . Three levels were evaluated for each variable: relative noise as 0, 1, and 2 standard deviations for both 237 process and observation uncertainty, amplitude of diel biological DO as 0, 1, and 2 mg L^{-1} , and 238 DO change from tidal advection as 0, 1, and 2 mg L^{-1} . A total of 81 time series were created 239 based on the unique combinations of parameters (Fig. 2). Half-window widths (day, hour of day, 240 and tide height) for the weighted regressions were evaluated for each time series: time as 1, 3, and 241 6 days, time of day as 1, 3, and 6 hours, and tidal height as 0.25, 0.5, and 1 as a proportion of the 242 total range given the height at the center of the window. The window widths were chosen based 243 on preliminary assessments that suggested a large range in model performance was described by

these values. In total, 27 window width combinations were evaluated for each of 81 simulated time series, producing results for 2187 weighted regressions.

The filtered DO time series were compared to the simulated data to evaluate the ability of 247 weighted regression to characterize the biological DO time series in eq. (4). Comparisons were made using Pearson correlation coefficients and the root mean square error (RMSE). Overall, the 249 weighted regressions produced filtered time series that were similar to the 'true' biological time 250 series regardless of the simulation parameters (Table 1) or window widths (Table 2, results for 251 each simulation can be viewed using the link in the multimedia section). The median correlation 252 between the filtered and biological values for all time series and window widths was 0.63, with 253 values ranging from 0.05 (very poor) to 1.00 (perfect). Mean error was 1.02, with values ranging 254 from 0 (perfect) to 2.12 (very poor). Simulations with very poor performance were those those 255 with the DO signal composed entirely of noise from observation uncertainty. As expected, 256 simulations with no biological or tidal influence had filtered time series that were identical to the 257 true time series (e.g., correlation of one, RMSE of zero). 258

Characteristics of DO time series that contributed to improved model performance were increasing amplitude of the diel DO component (DO_{die}) and increasing process error (e_{pro}), whereas increasing observation error contributed to decreased performance (Table 1 and Fig. 3). Model performance was not significantly affected by increasing tidal effects (i.e., increasing magnitude of DO_{adv}). Model performance was not substantially affected by variation in half window widths relative to characteristics of the DO time series (Table 2 and Fig. 4). Graphical summaries of model performance averaged by simulation parameters (Fig. 3) and half window widths (Fig. 4) support the general trends described by Tables 1 and 2.

Validation of weighted regression with case studies

Results from the simulated time series were used to inform the validation of weighted 268 regression with real data, specifically with respect to choosing half-window widths described 269 below. Continuous monitoring data from the National Estuarine Research Reserve System was used to validate the weighted regression model by evaluating estimates of ecosytem metabolism obtained from observed and filtered DO time series. NERRS is a federally-funded network of 28 protected estuaries established for long-term research, water-quality monitoring, education, and 273 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, CDMO 2014). 275 In addition to providing a basis for trend evaluation, data from SWMP provides an ideal opportunity to evaluate long-term variation in water quality parameters from biological and 277 physical processes. Continuous SWMP data can be used to describe DO variation at sites with different characteristics, including variation from ranges in tidal regime (Sanger et al. 2002) and 279 rates of ecosystem production (Caffrey 2003, 2004). We selected sites from the SWMP database 280 that had desirable characteristics for validating weighted regression. Specifically, four macrotidal 281 sites were chosen based on apparent relationships between DO and tidal changes (Fig. 5 282 and Table 3): Vierra Mouth station at Elkhorn Slough (ELKVM, California, 36.81°N, 121.78°W), 283 Bayview Channel at Padilla Bay (PDBBY, Washington, 48.50°N 122.50°W), Middle Blackwater 284 River station at Rookery Bay (RKBMB, Florida, 25.93°N 81.60°W), and Dean Creek station at 285 Sapelo Island (SAPDC, Georgia, 31.39°N 81.28°W). The ELKVM station is located at the mouth 286 of the Elkhorn Slough estuary in approximately four meters of water (mean low water depth). Bottom substrates are composed of compacted mud and sand due to large tidal influences. The

PDBBY station is located along the Bayview Channel, which is a major tributary of Padilla Bay that drains intertidal flats that include eelgrass beds and macroalgae. The site is in 1.5 meters of water (mean low low water) with bottom substrates composed of fine silt and clay overlying sand. 29 The RKBMB station is located at the mouth of the Middle Blackwater River in approximately 2 292 meters of water (mean high water depth). Salinity varies immensely with values ranging from 2.3 293 to 38.6 ppt throughout the year. Bottom substrates are a mixture of sand, silt, oyster shell, and 294 organic matter. Finally, the SAPDC station is located in Dean Creek, a small tidal basin that is fed 295 from the Doboy Sound on the south end of Sapelo Island. Mean low water depth is approximately 296 one meter and bottom substrates consist of sand and mud with occasional osyter reefs. 297

The weighted regression model was applied to continuous DO time series and water level 298 measurements from January 1st to December 31st 2012 at the four sites. Tide predictions were 299 obtained for each site using harmonic regression applied to the sonde depth data (oce package in 300 R, Foreman and Henry 1989, RDCT 2014). The predicted time series of tidal height from the 301 regressions were used for all models to avoid issues with missing values in the observed data. The 302 stations were generally semidiurnal or mixed semidiurnal and net heterotrophic on an annual 303 basis (Table 3). Net heterotrophy (i.e., respiration exceeding production) is typical for shallow 304 water systems at temperate latitudes (Caffrey 2003), although values in Table 3 were from 305 observed DO time series that were strongly correlated with water level height.

Estimates of ecosystem metabolism before and after filtering

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The weighted regression method was applied to the annual data for each station to obtain a
filtered DO time series for estimating metabolism. Ecosystem metabolism was estimated using
the open-water technique (Odum 1956) as described in Caffrey et al. (2014). The method is used

to infer net ecosystem metabolism using the mass balance equation:

$$\frac{\delta DO}{\delta t} = P - R + D \tag{14}$$

where the change in DO concentration (δDO , g O_2 m⁻³) over time (δt , hours) is equal to photosynthetic rate $(P, g O_2 m^{-3} hr^{-1})$ minus respiration rate $(R, g O_2 m^{-3} hr^{-1})$, corrected for air-sea gas exchange $(D, g O_2 m^{-3} hr^{-1})$ (Caffrey et al. 2014). D is estimated as the difference between the DO saturation concentration and observed DO concentration, multiplied by a volumetric reaeration coefficient, k_a (Thébault et al. 2008). The diffusion-corrected DO flux 316 estimates were averaged during day and night for each 24 hour period in the time series, where 317 flux is an hourly rate of DO change. Respiration rates were assumed constant during day and 318 night such that total daily rates were calculated as hourly respiration multiplied by 24. The 319 'metabolic day' was considered the approximate 24 hour period between sunsets on two adjacent 320 calendar days. Respiration was subtracted from daily net production estimates to yield gross 321 production (Table 3). 322

The selection of half-window widths for filtering the DO time series was based on an
evaluation of results using four performance metrics. In other words, the 'optimal' window
widths for each case study were those that provided the greatest measure of performance based on
all four metrics. First, the regression results were evaluated using correlations of DO and
metabolism estimates with tidal height before and after application of the model, such that
window widths that provided maximum reduction in correlation relative to the observed data were
desirable. Daily metabolism estimates before and after filtering were compared to the mean rate
of tidal height change (i.e., first derivative of the predicted tidal height) for each day during

separate solar periods. Production rates were compared to mean rates of tidal height change during the day and respiration rates were compared to mean rates of change during the night. The second and third performance metrics evaluated changes in the mean annual metabolism 333 estimates and standard deviation before and after filtering. We assumed that mean values that 334 represent annual aggregations would not change because tidal variation is primarily diurnal, 335 whereas the variance would be reduced by some amount after filtering. Optimum window widths 336 in this context were considered those that maintained the mean values while reducing standard 337 deviation relative to the observed data. Finally, results were evaluated based on the occurrence of 338 'anomalous' daily production or respiration estimates, where anomalous was defined as negative 339 gross production during the day and positive respiration estimates during the night. Anomalous 340 values have been previously attributed to the effects of physical processes on DO time series 341 (Caffrey 2003). Optimum window widths for this metric were those that provided the maximum 342 reduction in anomalous values. Although anomalies could be caused by processes other than tidal 343 advection, e.g., abiotic dark oxygen production (Pamatmat 1997), we assumed that physical 344 processes were the dominant sources of these values given the tidal characteristics at each site. 345 Multiple combinations of half-window widths were evaluated for the case studies. 346 Specifically, half-window widths of 1, 3, 6, 9, and 12 days, 1, 3, 6, 9, and 12 hours, and 0.2, 0.4, 347 0.6, 0.8, and 1 tidal height proportions were evaluated, producing a total of 125 unique combinations. Half-window widths that maximized the four performance metrics for each case study were chosen as the 'optimal' values. Accordingly, the optimal half-window widths were 12, 350 6, and 0.8 (days, hours, tidal height) for Elkhorn Slough, 3, 6, and 0.6 for Padilla Bay, 3, 1, and 351 0.6 for Rookery Bay, and 3, 1, and 0.6 for Sapelo Island. Filtering had significant effects on the 352 correlations between water level changes, DO time series, and daily integrated metabolism 353

estimates (Table 4, see the link in the multimedia section for graphical results of each case study).

Correlations of observed DO time series with predicted tidal height were positive at all sites,

except Padilla Bay where increases in water level were associated with decreases in DO

concentration. The filtered DO time series had correlations with tidal height close to zero.

Similarly, metabolic rates (production, respiration) estimated from the filtered DO time series had

significantly reduced correlations with tidal height change.

The percentage of daily integrated metabolism estimates that were anomalous (negative 360 production, positive respiration) were significantly reduced for all sites after filtering (Table 5), 361 perhaps indicating the relative effects of water movement. Before filtering, anomalous values 362 ranged from 9.15 (as a percentage of the total estimates, Rookery Bay) to 21.80 (Padilla Bay) for 363 production and 7.57 (Rookery Bay) to 20.68 (Elkhorn Slough) for respiration. Anomalous values 364 were reduced to near zero for all case studies, particularly Rookery Bay and Sapelo Island. 365 Metabolism estimates using filtered DO time series had decreased mean production (-63.1 % 366 change from the annual mean) and respiration (-62.6 %) for Elkhorn Slough, increased mean 367 production (17.8 %) and respiration (18.8 %) for Padilla Bay, and generally unchanged mean 368 production and respiration for Rookery Bay and Sapelo Island (Table 5). Changes in mean 369 estimates based on filtered DO time series suggests that the weighted regression removed 370 variation attributed to both biological and physical processes. The implications of these undesirable results are described below. Decreases in the standard deviation for all metabolism estimates were observed for all cases after filtering. However, reduction in variation may also 373 occur if the biological signal is reduced individually or in addition to physical variation. The extent to which this reduction is related to the former should be minimal, provided that the two 375 are statistically distinguishable. Situations when the phasing of the tidal and solar cycles are

correlated could be instances when the two are unable to be separated by the model. Reductions in mean annual values (particularly at Elkhorn Slough) in addition to variance reduction suggests that true metabolism may have been removed.

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An example from Sapelo Island illustrates the effects of weighted regression on DO and 380 metabolism estimates (Figs. 6 to 8). A two-week period in February showed when the tidal cycles 381 were both in and out of phase with the diel cycling, where phasing describes synchronicity 382 between maximum tide heights and day/night periods (Nidzieko et al. 2014). That is, maximum 383 tide heights were generally out of phase with the diel cycle during the first week when low tides 384 were observed during the middle of the night and the middle of the day (Fig. 6), whereas tide 385 heights were in phase during the second week when the maximum tide height occured during the 386 day and night (Fig. 7). The effects of tidal height change on the observed DO time series are 387 visually apparent in the plots. The first week illustrates a strong negative bias (less respiration, 388 less production) in the observed DO signal from low tides at mid-day and mid-night, whereas the 389 second example illustrates a strong positive bias (more respiration, more production) in the 390 observed DO from high tides. These biases are apparent in the metabolism estimates using the 39 observed data (Fig. 8). Anomalous estimates occur when low tides are in phase with the solar 392 cycle (week one), whereas metabolism estimates are likely over-estimated when high tides are in 393 phase with the solar cycle (week two). The filtered time series shows noticeable changes given the direction of bias from the phasing between tidal height and diel period. DO values were higher after filtering when low tides occurred during night and day periods, whereas DO values were lower after filtering when high tides occurred during day and night periods (Figs. 6 and 7). 397 Changes in metabolism estimates after filtering were also apparent, such that the anomalous 398 values were removed during the first week and the positive bias in the second week is decreased 399

400 (Fig. 8).

401 Accuracy of results and effects of aggregation

A point of concern is the period of observation within which observed DO is affected by 402 tidal height changes and the extent to which this affects the interpretation of ecosystem metabolism. The effects of tidal variation on daily estimates may not be of concern if seasonal or annual aggregations (e.g., mean annual metabolism) remove this potential bias. The example from Sapelo Island in the previous section highlights this point given that mean production and respiration estimates before and after filtering were generally unchanged for the two-week period. 407 Alternatively, annual averages of production and respiration estimates were significantly different for Elkhorn Slough and Padilla Bay but not Rookery Bay and Sapelo Island (Table 5). Therefore, 409 an evaluation of weighted regression to filter the effects of tidal variation on ecosystem 410 metabolism for different periods of observation is critical for its application. Specifically, does the 411 period of observation affect the ability of weighted regression to remove physical variation in the 412 time series? When should filtering be applied if aggregation of observed data on longer time 413 periods removes potential bias? The first question is addressed by evaluating collinearity between 414 tidal change and solar periods. The second question is addressed by comparing observed and 415 filtered estimates that are aggregated over different periods of observation. 416

Collinearity between tidal height change and solar cycling likely affected the ability of
weighted regression to quantify the variation in DO time series. Model parameterization may be
unreliable if, for example, tidal height follows diurnal periods by increasing during the day or
decreasing during the night. Nidzieko et al. (2014) found that such covariation is common in
Elkhorn Slough during the summer months when high tides always occurred during the night.

Given that the phasing between tidal height change and diurnal cycling is variable, the ability of weighted regression to quantify variation attributed to both is also expected to vary. The correlation between sun angle and tidal change (measured as an angular rate) was evaluated using 424 a moving window approach for each case study. This approach is analogous to weighted 425 regression by providing an indication of when collinearity may occur as a function of the moving 426 window. Weighted regression can be expected to effectively characterize biological and physical 427 variation during periods when the correlation between tidal height change and diurnal cycling is 428 low within the window. Fig. 9 suggests that collinearity between sun angle and tidal height 429 change can exceed +/-0.2 for Elkhorn Slough and Padilla Bay, whereas correlations were much 430 smaller regardless of the period of observation for Rookery Bay and Sapelo Island. Given the 431 change in mean annual metabolism using the filtered DO time series and the relatively high 432 collinearity between tidal change and solar cycling, the results for Elkhorn Slough and Padilla 433 Bay may not be accurate. The results may only be interpretable when correlations are close to 434 zero (e.g., April and October for Elkhorn Slough). 435

The observed and filtered daily estimates were averaged by month for each case study to
evaluate effects of aggregation on mean production and respiration, in addition to the mean
annual estimates in Table 5. Significant variation in aggregated production and respiration
estimates was observed for each case study (Fig. 10). Filtered production and respiration
estimates for Padilla Bay and Rookery Bay exhibited monthly variation that was more
characteristic of expected trends during warmer months. Specifically, metabolism estimates based
on observed DO were substantially muted for both Padilla Bay and Rookery Bay during summer
months, whereas values were significantly higher after filtering. Results for Sapelo Island
suggested that aggregated estimates were similar before and after filtering, although winter and

summer months were slightly under- and over-estimated, respectively, using the observed data.

Results for Elkhorn Slough varied significantly such that production and respiration were

significantly reduced after filtering, which may have been related to collinearity. Overall, these

trends emphasize the importance of considering different aggregation periods for interpreting

metabolism estimates. Each case study showed differences in observed and filtered values at

monthly aggregations, suggesting tidal variation may influence metabolism estimates at relatively

long time scales Table 5).

Discussion

The weighted regression approach was developed to improve estimates of ecosystem 453 metabolism by removing variation associated with tidal change in observed DO time series. The 454 application to simulated DO time series with known characteristics and extension to continuous monitoring data from selected NERRS sites suggested the approach can isolate and remove variation in observed DO from tidal change. Further, aggregation of metabolism estimates using the filtered DO time series were significantly different than those using the observed data, 458 particularly for relatively long periods of observation depending on location. These results 459 suggest that previous estimates may not accurately reflect true metabolic signals if the effects of 460 tidal variation confound biological signals in observed DO time series. Additionally, variation of 461 aggregated metabolism estimates were substantially reduced after filtering, suggesting greater 462 confidence in interpreting estimates even if the mean values are similar. 463

Comparisons between filtered and biological DO time series from the simulations indicated that weighted regression can reduce the effects of tidal variation for a range of characteristics of DO time series. An examination of scenarios that produced abnormal results

can provide additional insight into factors that affect the performance of weighted regression. For example, poor performance was observed when the observation uncertainty (ϵ_{obs}) was high and both process uncertainty (ϵ_{pro}) and tidal advection (DO_{adv}) were low. These examples represent time series with excessive random variation, no auto-correlation, and no tidal influence. Poor performance is expected because the weighted regression models a non-existent tidal signal in a 471 very noisy DO time series. These results were observed even for time series with a large diel 472 component of the biological DO signal, suggesting that the model will produce random results in 473 microtidal systems with high noise and no serial correlation. From a practical perspective, 474 weighted regression should not be applied to noisy time series if there is not sufficient evidence to 475 suggest the variation is related to tidal changes. Alternative approaches, such as the Kalman filter (Harvey 1989, Batt and Carpenter 2012), may be more appropriate if random variation is the 477 primary source of uncertainty. Similarly, results with perfect or near-perfect correlations between 478 filtered and biological DO time series were observed when observation uncertainty and tidal 479 effects were not components of the simulated time series. Although there is no need to apply 480 weighted regression to time series with no apparent tidal influences, the results will not be 48 incorrect. We emphasize that the weighted regression should only be applied to time series for 482 which specific conditions apply, as described in the recommendations below. 483

For all case studies, weighted regression was generally successful in reducing the
variation in the DO time series that was presumably caused by physical advection. In particular,
the reduction of anomalous metabolism estimates after filtering was observed. Negative
production and positive respiration estimates suggest assumptions of the open-water method are
violated (Needoba et al. 2012), although 'normal' estimates (positive production and negative
respiration) may still include a significant source of bias from physical advection by providing

over-estimates of true values. For example, Nidzieko et al. (2014) observed that net metabolism at
Elkhorn Slough was strongly heterotrophic during spring tides that occurred at nighttime such
that inundation of salt marshes during the night followed by draining with low tide during the day
lead to inflated respiration values. Such measurements are not necessarily 'incorrect' estimates of
metabolism, although they may not be easily assigned to discrete locations without empirical data
on lateral water movements. Synchrony between solar and tidal cycles is a critical concern for
interpreting metabolism estimates such that collinearity between the two may diminish the
performance of weighted regression.

The weighted regression approach makes no assumptions as to the relationships between 498 DO and tidal variation over time. Although the functional form of the model is a simple linear 499 regression with only two explanatory variables (eq. (1)), the moving window approach combined 500 with the adaptive weighting scheme allows for quantification of complex tidal effects that may not 501 be possible using alternative approaches. A similer approach by Batt and Carpenter (2012) uses a 502 Kalman filter to improve estimates of ecosystem metabolism in lakes. The approach minimizes 503 uncertainty in observed DO using a filter that combines information about the data generation 504 process and the manner in which the data are observed (Harvey 1989). Although a similar 505 approach could be used for estuaries, it may not be effective given that tidal advection may not be 506 related to process or observation uncertainty as they are defined. Additionally, results from the case studies illustrated the ability of the weighted regression approach to model changes over time in the relationships between tidal change and DO. Results for Padilla Bay and Rookery Bay suggested that filtering had the largest effect during the summer, whereas the results for cooler months were not significantly different from the observed. The weighted regression method 511 produced filtered time series that accommodated seasonal variation in DO conditional on tidal

height change, whereas moving window filters or standard regression techniques would likely not
have characterized these dynamic relationships.

Comments and recommendations

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Results from the simulations and case studies suggested that weighted regression can be a 516 practical approach for filtering DO time series. However, application may only be appropriate 517 under specific situations. The case studies were chosen based on the relatively high percentage of 518 metabolism estimates that were anomalous and the strength of correlation between the observed 519 DO time series and tidal height. Despite these similarities, filtering had variable effects on 520 metabolism estimates. The results for Elkhorn Slough and Padilla Bay are of particular concern 521 given that mean annual estimates were substantially different compared to those from the 522 observed DO time series. Although the correlation of DO and tidal height was reduced for both cases, in addition to a reduction of anomalous estimates, collinearity between tidal change and solar cycling likely contributed to the relative change in mean metabolism before and after filtering. Evaluating collinearity, as in Fig. 9, is an important diagnostic for characterizing the 526 expected performance of weighted regression and choosing appropriate window widths. These 527 plots should indicate whether weighted regression is appropriate for the whole time series (e.g., 528 Sapelo Island) or only for specific periods when collinearity is low (e.g., April and October at 529 Elkhorn Slough). 530

DO time series that include components of metabolism related to diurnal cycling as well as true biological effects related to the tide should be evaluated with caution. Specifically, increased respiration may be observed during ebb tides as a result of increased enrichment of substrates (Sasaki et al. 2009). In such cases, variation in the metabolic signal is correlated and

directly related to the tide but is not related to physical movement of water masses. Accordingly, the model should not be used without critical evaluation of site-level characteristics that suggest physical movement of water masses is a primary source of noise in a DO signal. Locations where 537 tidal influences are large and the water is relatively deep (as in the Vierra Mouth station at Elkhorn Slough) are clear examples where physical movement is likely the dominant source of 539 variation in the DO signal. Application to stations where this is less clear should be carefully evaluated, particularly with respect to changing window widths on the results. In general, the 541 results should be evaluated using multiple performance metrics as above. The optimal window widths are likely those that reduce anomalous metabolism estimates, minimize correlations 543 between observed DO and tide height, and reduce clear visual patterns of tide change on DO. In 544 general, a pragmatic approach is emphasized such that results should be evaluated based on the 545 preservation of diel variation from production while exhibiting minimal changes with the tide. 546 Such an approach, combined with further validation, will support informed management 547 decisions through more accurate estimates of ecosystem metabolism.

References

- Batt RD, Carpenter SR. 2012. Free-water lake metabolism: Addressing noisy time series with a Kalman filter. Limnology and Oceanography: Methods, 10:20–30.
- Caffrey JM. 2003. Production, respiration and net ecosystem metabolism in U.S. estuaries. Environmental Monitoring and Assessment, 81(1-3):207–219.
- Caffrey JM. 2004. Factors controlling net ecosystem metabolism in U.S. estuaries. Estuaries, 27(1):90–101.
- Caffrey JM, Murrell MC, Amacker KS, Harper J, Phipps S, Woodrey M. 2014. Seasonal and
 inter-annual patterns in primary production, respiration and net ecosystem metabolism in 3
 estuaries in the northeast Gulf of Mexico. Estuaries and Coasts, 37(1):222–241.
- CDMO (Centralized Data Management Office). 2014. National Estuarine Research Reserve
 System. http://cdmo.baruch.sc.edu/. (Accessed January, 2014).
- Collins JR, Raymond PA, Bohlen WF, Howard-Strobel MM. 2013. Estimates of new and total productivity in Central Long Island Sound from in situ measurements of nitrate and dissolved oxygen. Estuaries and Coasts, 36(1):74–97.
- Coloso JJ, Cole JJ, Pace ML. 2011. Difficulty in discerning drivers of lake ecosystem metabolism with high-frequency data. Ecosystems, 14(6):935–948.
- Cryer JD, Chan KS. 2008. Time Series Analysis with Applications in R. Springer, New York,
 New York, second edition.
- D'Avanzo C, Kremer JN, Wainwright SC. 1996. Ecosystem production and respiration in response to eutrophication in shallow temperate estuaries. Marine Ecology Progress Series, 141(1-3):263–274.
- Foreman MGG, Henry RF. 1989. The harmonic analysis of tidal model time series. Advances in Water Resources, 12(3):109–120.
- Harvey AC. 1989. Forecasting, Structural Time Series Models and the Kalman Filter. Cambridge
 University Press, Cambridge, United Kingdom.
- Hilborn R, Mangel M. 1997. The Ecological Detective: Confronting Models with Data.
 Princeton University Press, Princeton, New Jersey.
- Hirsch RM, Moyer DL, Archfield SA. 2010. Weighted regressions on time, discharge, and season (WRTDS), with an application to Chesapeake Bay river inputs. Journal of the American Water Resources Association, 46(5):857–880.
- Kemp WM, Boynton WR. 1980. Influence of biological and physical processes on dissolved
 oxygen dynamics in an estuarine system: Implications for the measurement of community
 metabolism. Estuarine and Coastal Marine Science, 11(4):407–431.

- Kemp WM, Testa JM. 2012. Metabolic balance between ecosystem production and consumption.
- In: Wolanski E, McLusky DS, editors, Treatise on Estuarine and Coastal Science, pages
- 83–118. Academic Press, New York.
- Needoba JA, Peterson TD, Johnson KS. 2012. Method for the quantification of aquatic primary
- production and net ecosystem metabolism using in situ dissolved oxygen sensors. In:
- Tiquia-Arashiro SM, editor, Molecular Biological Technologies for Ocean Sensing, pages
- ⁵⁸⁹ 73–101. Springer, New York.
- Nidzieko NJ, Needoba JA, Monismith SG, Johnson KS. 2014. Fortnightly tidal modulations affect net community production in a mesotidal estuary. Estuaries and Coasts.
- Nixon SW. 1995. Coastal marine eutrophication: A definition, social causes, and future concerns.
 Ophelia, 41:199–219.
- NRC (National Research Council. 2000. Clean Coastal Waters: Understanding and Reducing the Effects of Nutrient Pollution. National Academy Press, Washington, DC.
- Odum HT. 1956. Primary production in flowing waters. Limnology and Oceanography, 1(2):102–117.
- Pamatmat MM. 1997. Non-photosynthetic oxygen production and non-respiratory oxygen uptake in the dark: A theory of oxygen dynamics in plankton communities. Marine Biology, 129(4):735–746.
- RDCT (R Development Core Team). 2014. R: A language and environment for statistical computing, v3.1.0. R Foundation for Statistical Computing, Vienna, Austria. http://www.R-project.org.
- Russell MJ, Montagna PA. 2007. Spatial and tepmoral variability and drivers of net ecosystem metabolism in western Gulf of Mexico estuaries. Estuaries and Coasts, 30(1):137–153.
- Sanger DM, Arendt MD, Chen Y, Wenner EL, Holland AF, Edwards D, Caffrey J. 2002. A
 synthesis of water quality data: National estuarine research reserve system-wide monitoring
 program (1995-2000). Technical report, National Estuarine Research Reserve Technical Report
 Series 2002:3. South Carolina Department of Natural Resources, Marine Resources Division
 Contribution No. 500, Charleston, South Carolina.
- Sasaki A, Hagimori Y, Nakatsubo T, Hoshika A. 2009. Tidal effects on the organic carbon mineralization rate under aerobic conditions in sediments of an intertidal estuary. Ecological Research, 24(4):723–729.
- Shumway RH, Stoffer DS. 2011. Time Series Analysis and its Applications: With R Examples.
 Springer, New York, New York, 3rd edition.
- Staehr PA, Bade D, de Bogert MCV, Koch GR, Williamson C, Hanson P, Cole JJ, Kratz T. 2010.
- Lake metabolism and the diel oxygen technique: State of the science. Limnology and
- Oceanography: Methods, 8:628–644.

- Thébault J, Schraga TS, Cloern JE, Dunlavey EG. 2008. Primary production and carrying capacity of former salt ponds after reconnection to San Francisco Bay. Wetlands, 28(3):841–851.
- Tukey JW. 1977. Exploratory Data Analysis. Addison-Wesley, Reading, Massachusetts.
- Wenner E, Sanger D, Arendt M, Holland AF, Chen Y. 2004. Variability in dissolved oxygen and
 other water-quality variables within the National Estuarine Research Reserve System. Journal
 of Coastal Research, 45(SI):17–38.
- Ziegler S, Benner R. 1998. Ecosystem metabolism in a subtropical, seagrass-dominated lagoon.
 Marine Ecology Progress Series, 173:1–12.

Figures

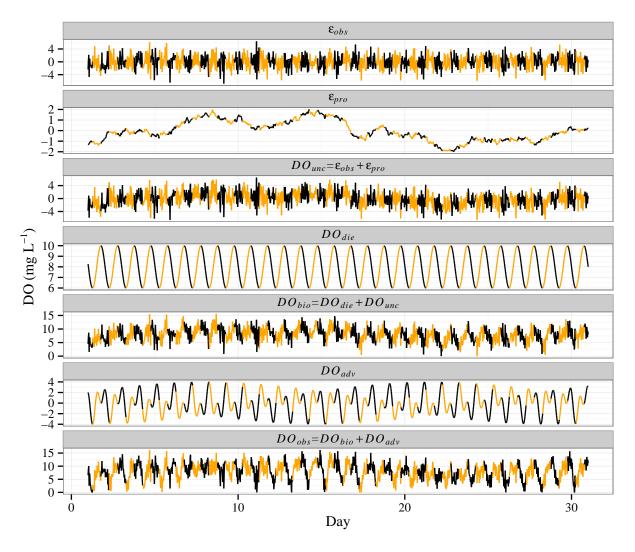


Fig. 1: Example of each component of a simulated DO time series for testing weighted regression. The time series were created using eqs. (4) to (13). Yellow indicates a twelve hour daylight period beginning at 630 each day.

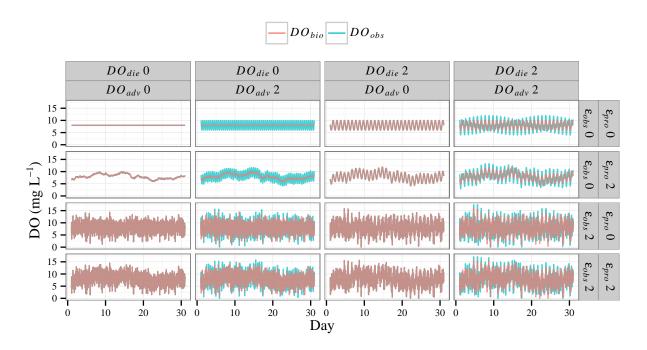


Fig. 2: Representative examples of simulated time series of observed DO (DO_{obs} , blue lines) and biological DO (DO_{bio} , as a component of observed, red lines) created by varying each of four parameters: strength of tidal association with DO signal (DO_{adv}), amount of process uncertainty (ϵ_{pro}), amount of observation uncertainty (ϵ_{obs}), and strength of diel DO component (DO_{die}). Parameter values represent the minimum and maximum used in the simulations as mg L⁻¹ of DO.

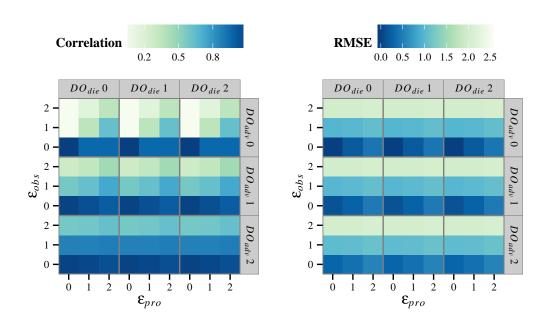


Fig. 3: Heat maps of correlations and errors (RMSE) for filtered DO time series (DO_{dtd}) from weighted regression with 'true' biological DO (DO_{bio}) for varying simulation parameters: strength of tidal association with DO signal (DO_{adv}), amount of process uncertainty (ϵ_{pro}), amount of observation observation uncertainty (ϵ_{obs}), and strength of diel DO component (DO_{die}). Each tile represents the correlation or error from results for a given combination of simulation parameters averaged for all window widths (as in Fig. 4).

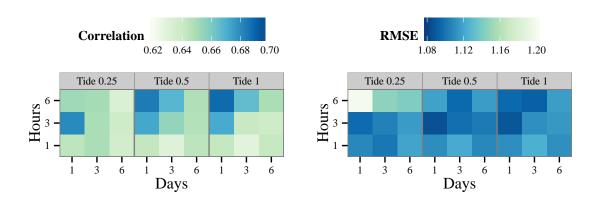


Fig. 4: Heat maps of correlations and errors (RMSE) for filtered DO time series (DO_{dtd}) from weighted regression with 'true' biological DO (DO_{bio}) for varying half window widths: days, hour of day, and proportion of tidal range. Each tile represents the correlation or error from results for a given combination of window widths averaged for all simulation parameters (as in Fig. 3).



Fig. 5: Locations of NERRS sites used as case studies to validate weighted regression. Stations at each reserve are ELKVM (Vierra Mouth at Elkhorn Slough), PDBBY (Bayview Channel at Padilla Bay), RKBMB (Middle Blackwater River at Rookery Bay), and SAPDC (Dean Creek at Sapelo Island).

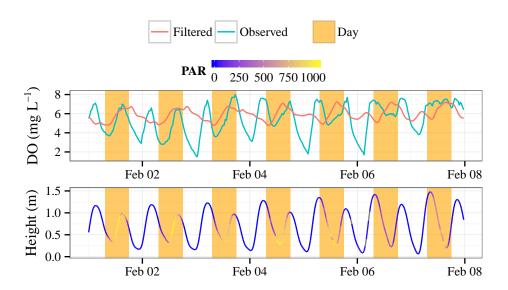


Fig. 6: Continuous DO time series before (observed) and after (filtered) filtering with weighted regression (top) and tidal height (m) colored by total photosynthetically active radiation (bottom, mmol m⁻²). Results are for the Sapelo Island station for a seven day period when high tide events were out of phase with diel periods, creating lower than expected observed DO during night and day periods. Filtered values are based on a weighted regression with half window widths of six days, one hour within each day, and tidal height proportion of one half.

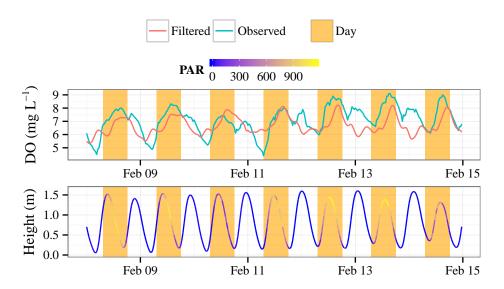


Fig. 7: Continuous DO time series before (observed) and after (filtered) filtering with weighted regression (top) and tidal height (m) colored by total photosynthetically active radiation (bottom, mmol m⁻²). Results are for the Sapelo Island station for a seven day period when high tide events were in phase with diel periods, creating higher than expected observed DO during night and day periods. Filtered values are based on a weighted regression with half window widths of six days, one hour within each day, and tidal height proportion of one half.

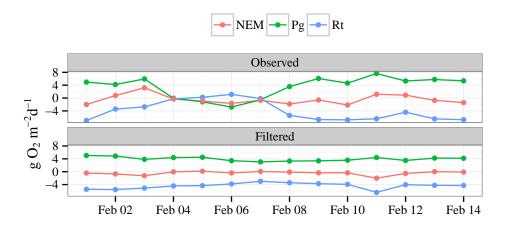


Fig. 8: Example of daily mean metabolism (net ecosystem metabolism, gross production, and total respiration) before (observed) and after (filtered) filtering with weighted regression. Results are for the Sapelo Island station for a two week period in February, 2012 when high tide was out of phase with the diel cycle during the first week (Fig. 6) and in phase during the second week (Fig. 7).

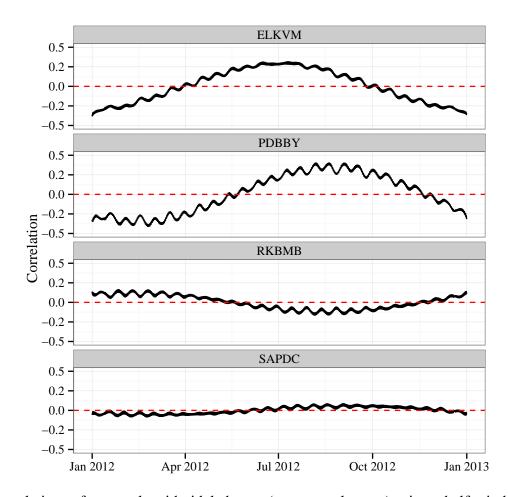


Fig. 9: Correlations of sun angle with tidal change (as an angular rate) using a half-window width of 12 days. Correlations larger or smaller than zero are periods when weighted regression may not effectively quantify variation from biological and physical sources in DO time series due to collinearity.

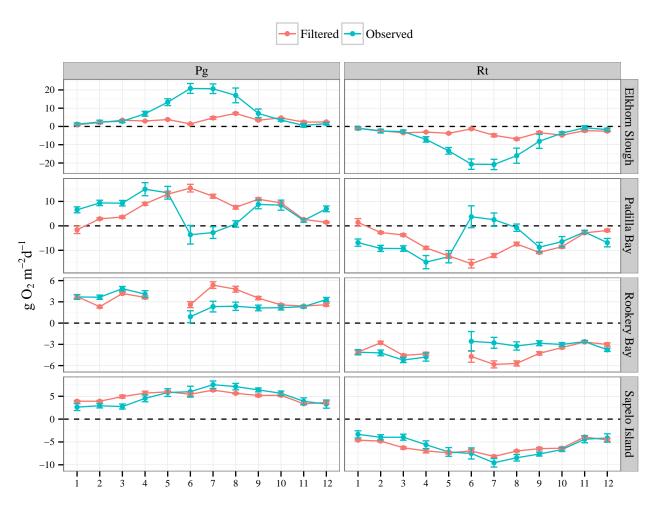


Fig. 10: Means and standard errors of daily metabolism estimates (gross production, total respiration) aggregated by month. Aggregated estimates are shown for observed and filtered DO time series. May was removed from Rookery Bay because of incomplete data.

629 Tables

Table 1: Summary (range, median, quartiles) of correlations and error estimates comparing filtered and biological DO time series for different simulation parameters (DO_{die} , DO_{adv} , ϵ_{pro} , ϵ_{obs}). Values represent averages from multiple simulations with common parameters. For example, row one is a summary of all simulations for which the diel DO component was zero (n = 729).

Parameter	Correlation						RMSE					
	Min	25^{th}	Median	75 th	Max	_	Min	25 th	Median	75 th	Max	
$\overline{DO_{die}}$												
0	0.05	0.20	0.41	0.86	1.00		0.00	0.33	1.01	1.96	2.05	
1	0.28	0.44	0.61	0.93	1.00		0.02	0.42	1.02	1.96	2.06	
2	0.55	0.60	0.81	0.96	1.00		0.05	0.52	1.06	1.99	2.12	
$\overline{DO_{adv}}$												
0	0.05	0.42	0.63	0.93	1.00		0.00	0.46	1.02	1.97	2.12	
1	0.05	0.42	0.63	0.93	1.00		0.00	0.46	1.02	1.97	2.12	
2	0.05	0.42	0.63	0.93	1.00		0.00	0.46	1.02	1.97	2.12	
$\overline{\epsilon_{pro}}$												
0	0.05	0.31	0.58	0.99	1.00		0.00	0.23	0.99	1.95	2.11	
1	0.16	0.37	0.61	0.93	0.99		0.10	0.33	1.02	1.97	2.11	
2	0.34	0.58	0.69	0.89	0.98		0.19	0.56	1.10	2.01	2.12	
ϵ_{obs}												
0	0.80	0.93	0.97	0.99	1.00		0.00	0.17	0.29	0.46	0.84	
1	0.05	0.56	0.62	0.81	0.84		0.97	1.00	1.02	1.08	1.28	
2	0.05	0.31	0.38	0.57	0.63		1.93	1.97	1.98	2.01	2.12	

Table 2: Summary (range, median, quartiles) of correlations and error estimates comparing filtered 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 averages from multiple simulations with common window values For example, row one is a summary of all simulations for which the half window width was one day (n = 729).

Window	Correlation					RMSE					
	Min	25^{th}	Median	75 th	Max	-	Min	25 th	Median	75 th	Max
Days											
1	0.07	0.44	0.66	0.96	1.00		0.00	0.43	1.02	1.96	2.12
3	0.07	0.41	0.62	0.93	1.00		0.00	0.45	1.02	1.97	2.08
6	0.05	0.37	0.61	0.88	1.00		0.00	0.51	1.02	1.97	2.08
Hours											
1	0.07	0.38	0.61	0.89	1.00		0.00	0.51	1.02	1.97	2.05
3	0.06	0.42	0.63	0.95	1.00		0.00	0.43	1.02	1.97	2.05
6	0.05	0.44	0.64	0.95	1.00		0.00	0.48	1.04	1.96	2.12
Tide											
0.25	0.05	0.42	0.62	0.92	1.00		0.00	0.47	1.03	1.97	2.12
0.5	0.07	0.42	0.63	0.94	1.00		0.00	0.45	1.02	1.96	2.04
1	0.07	0.42	0.63	0.94	1.00		0.00	0.44	1.02	1.97	2.04

Table 3: Summary statistics of tidal component amplitudes (m), selected water quality parameters (DO mg L^{-1} , chlorophyll-a μ g L^{-1} , salinity psu, water temperature °C) 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). Water quality data are averages for the entire period of record for each site. Metabolism estimates are means of daily integrated values.

Site	Tidal amplitude				Water quality					Metabolism ^a			
	O1	P1	M2	S2		DO	Chl	Sal	Temp		Pg	Rt	NEM
ELKVM	0.24	0.12	0.48	0.13	,	7.87	3.87	32.43	13.78	8	.14	-8.19	-0.05
PDBBY	0.46	0.23	0.63	0.15	8	8.97	2.24	29.17	10.44	5	.95	-5.90	0.05
RKBMB	0.13	0.04	0.36	0.10	4	4.48	4.50	30.53	25.85	3	.02	-3.62	-0.60
SAPDC	0.10	0.02	0.54	0.07	4	4.96	5.98	27.30	21.77	4	.89	-6.04	-1.16

^aPg: gross production, Rt: respiration, NEM: net ecosystem metabolism

Table 4: Correlations of tidal changes at each site with continuous DO observations and metabolism estimates (gross production, respiration) before (observed) and after (filtered) filtering with weighted regression. Values are averages of monthly correlations. DO values are correlated with predicted tidal height at each observation, whereas metabolism estimates are correlated with mean tidal height change between observations during day or night periods for production and respiration, respectively.

Site	DO	Pg^a	Rt	
ELKVM				
Observed	0.44	0.43	0.43	
Filtered	-0.04	0.04	-0.01	
PDBBY				
Observed	-0.49	-0.11	-0.29	
Filtered	0.01	-0.05	0.00	
RKBMB				
Observed	0.45	0.26	0.34	
Filtered	0.02	-0.04	0.03	
SAPDC				
Observed	0.62	0.47	0.64	
Filtered	0.00	-0.04	0.07	

^aPg: gross production, Rt: respiration, NEM: net ecosystem metabolism

Table 5: Summary of metabolism estimates (gross production, respiration) for case studies using DO time series before (observed) and after (filtered) filtering with weighted regression. Means and standard deviation are based on daily integrated metabolism estimates. Anomalous values are the percentage of metabolism estimates that were negative for gross production and positive for respiration.

Site	$\mathbf{P}\mathbf{g}^a$			Rt				
	Mean	SD	Anom	Mean	SD	Anom		
ELKVM								
Observed	8.14	11.44	18.64	-8.19	11.82	20.68		
Filtered	3.00	2.26	6.78	-3.06	2.34	7.12		
PDBBY								
Observed	5.95	11.69	21.80	-5.90	12.60	19.03		
Filtered	7.01	6.85	4.84	-7.01	6.81	5.54		
RKBMB								
Observed	3.02	2.55	9.15	-3.62	2.65	7.57		
Filtered	3.46	1.79	0.63	-4.07	1.88	0.63		
SAPDC								
Observed	4.89	4.42	13.39	-6.04	4.78	10.93		
Filtered	4.94	1.74	0.00	-6.13	1.99	0.00		

^aPg: gross production, Rt: respiration

330 Multimedia

- The supporting information for this manuscript includes a graphical illustration of the
- weighting scheme described in the material and procedures section
- 633 (http://spark.rstudio.com/beckmw/weights_widget), results for each simulation
- 634 (http://spark.rstudio.com/beckmw/detiding_sims), and results for each case study
- 635 (http://spark.rstudio.com/beckmw/detiding_cases). Each link is a graphical summary of data
- based on interactive inputs to support the results in the manuscript.