



Fitting metabolic models to dissolved oxygen data: The Estuarine BAYesian Single-station Estimation method (EBASE)

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Abstract:	<p>Continuous measurements of dissolved oxygen (DO) are useful for quantifying ecosystem metabolism, which is critical for understanding estuarine biogeochemistry and ecology, but current methods applied to these data may lead to estimates that are physically impossible and poorly constrained errors. Here we present a new approach for estimating estuarine metabolism: EBASE (Estuarine BAYesian Single-station Estimation). EBASE applies a Bayesian framework to a simple process-based model and DO observations, allowing the estimation of critical model parameters, specifically light efficiency and respiration, as informed by a set of prior distributions. EBASE improves upon the stream-based model from which it was derived by accommodating missing DO data and allowing the user to set the time period over which parameters are estimated. We demonstrate that EBASE can recover known metabolic parameters from a synthetic time series, even in the presence of noise (e.g., due to tidal advection) and when prior distributions are uninformed. Optimization periods of 7 days and 30 days are more preferable than 1 day. A comparison with the more-conventional method of Odum reveals the ability of EBASE to avoid unphysical results (such as negative photosynthesis and respiration) and improves when the DO data are detided. EBASE is available using open-source software (R) and can be readily applied to multiple years of long-term monitoring data that are available in many estuaries. Overall, EBASE provides an accessible method to parameterize a simple metabolic model appropriate for estuarine systems and will provide additional understanding of processes that influence ecosystem status and condition.</p>



We thank all three reviewers for providing thorough and constructive comments that have helped to improve the manuscript. Our responses to each of these comments are provided below. Note that line numbers refer to those in the original manuscript.

Reviewer 1

This manuscript describes an advancement in the computation of aquatic estuarine metabolism (i.e., primary production and respiration) using open-water dissolved oxygen (DO) time series. The authors adapted a Bayesian model originally developed for non-tidal, lotic systems (i.e., BASE) to 1) now work with time series that have missing dissolved oxygen observations and 2) can accommodate longer time periods for metabolism estimates. The latter could produce non-real estimates of metabolism in earlier methods while the former is achieved through linear interpolation during pre-processing and estimate removal by a user defined threshold during post-processing. The authors describe in sufficient detail how to operationalize the model and provide a comparison with a historically more standard arithmetic-based model that has been used in earlier studies of estuarine metabolism. Furthermore, the authors provide an R package “EBASE” to allow others to estimate estuarine metabolism using this method advancement; a package I am sure the coastal community will find useful. Overall, this paper was well written and the advancement significant. This paper should be considered for publication in L&O Methods following incorporation of the comments below.

Response: Thank you for providing these thorough comments on our manuscript. Please see our responses below.

There were two studies cited in the introduction (Line 98) as having used Bayesian techniques to estimate aquatic metabolism in estuaries. Please elaborate on how the method described in this study is consistent with and/or different from those in the cited studies.

Response: We agree this clarification is needed. The first study (Ciavatta et al. 2008) actually did not use a Bayesian approach, rather it provided simultaneous estimation of the metabolic parameters using a conventional empirical model framework. This reference to a Bayesian approach was in error and we have removed this citation from the introduction. Tassone and Bukaveckas (2019) does provide a good example for comparison with our work and we elaborate on this in the revised text on line 105: “Tassone and Bukaveckas (2019) adapted a Bayesian approach developed for streams (Appling et al. 2018) in an estuarine setting to estimate metabolic rates in the James River. Although this approach demonstrated the utility of such an approach in estuaries, much of the core model structure developed for streams was unchanged and may not have been fully descriptive of fundamental processes influencing metabolism in open-water environments.”

We then continue the justification for our use of BASE, adding the following:

Line 108: “The underlying model components can also easily be updated given the relatively simple format of the approach.”

Line 115: “We focus on BASE given the relative simplicity and, therefore, ease of application compared to other stream-based Bayesian approaches (e.g., Appling et al. 2018).”

The streamMetabolizer package is a great contribution to the field, although our implicit goal of this work was to modify a readily accessible open source approach such as BASE for our needs. The framework was easily extendable for our chosen gas-exchange method (Wanninkhof 2014) and modification of the software functionality (i.e., user-chosen optimization period and dealing with data gaps).

The authors describe pitfalls in their model, particularly when it comes to estimating the gas transfer velocity. Additionally, the authors provide evidence that sometimes the right answer (i.e., modeled DO time series, lines 349-352) can be achieved through incorrect processes. Similar issues have been described and addressed in the stream metabolism literature which was not cited or discussed in this study, please see Appling et al. 2018 - <https://doi.org/10.1002/2017JG004140>). Consider adding to the discussion how EBASE might incorporate these advancements to address these issues.

Response: Thank you for pointing out this reference. We have included an explicit mention of equifinality and a citation for Appling et al. (2018) on line 352. Also please see our addition to the discussion on line 490. This is described in full in response to the general comments from Reviewer 3.

Detiding (i.e., removing the influence of tidal cycles on time series data) the DO time series substantially improved model estimates and therefore was recommended as a step prior to applying the model. However, it was not clear how the authors detided their time series (they used Weighted Regression but it is unclear how this method removes tidal influence from the predicted time series – see lines 400-402). Please add additional information on the detiding approach and which variables were detided (i.e., was only DO detided? Wouldn't all water-related input variables, such as water temperature and salinity, need to be detided?).

Response: The detiding approach used herein is thoroughly described in another L&O paper cited in the main text (Beck et al. 2015). Describing this approach in detail is beyond the scope of the paper, although we have added some text for clarification. Also, the method has only been applied to dissolved oxygen data, so we have not used it for any of the remaining parameters. Clarification for both points has been added to line 399: “The results of this analysis return a predicted and detided dissolved oxygen time series, where the detided results are simply the predictions at average tidal height (see Beck et al. 2015 for details). This method was only applied to dissolved oxygen since it has not been evaluated with any other parameters.”

How would your results be impacted by using different observed data collection frequencies such as every 5-min, 15-min, 1 hour?

Response: The resolution of “continuous” monitoring data has not been evaluated in this study, although our guess is that more frequent sampling may produce more robust estimates. However, this may not matter given the time scales at which metabolism changes (i.e., > 1 day). In our experience, estimates from the Odum open-water method are nearly identical using 15-minute or hourly samples. Not sure the same would apply for EBASE given the fundamental differences between the approaches. We have added a point in the discussion on line 541 that speaks to this question: “These hypotheses may also consider frequency of continuous monitoring (e.g., 15 minute vs hourly) and how this may influence the results, as this is currently unknown for EBASE.”

In my use of Bayesian models for estimating metabolism, with each model run you can get different metabolism estimates. This is due to the prior distribution space that the model can operate in. Is this something you have noticed with your model? If so, could you add a sentence somewhere explaining that a user should expect different modeled estimates with each model run?

Response: Surprisingly, we have not encountered this issue with EBASE. Obviously the results depend on the prior distributions, which was the purpose of our sensitivity analysis, although we have not noticed slightly different results for different runs with the same priors. It is possible these differences are present, but small enough not to notice. We would hope that a user of this approach would be familiar enough with Bayesian and MCMC methods to expect these minor differences.

Line 32-36: Estuaries are also significantly influenced by their freshwater end-members, consider adding ‘river’ to ‘...interface between land, river, ocean, and atmosphere’. Similarly consider incorporating rivers into ‘...transported from land to rivers to ocean...’.

Response: Added.

Line 47: Consider adding how materials are lost to the atmosphere, the sediments, and the ocean. For example, “...that are lost to the atmosphere (i.e., outgassing), the sediments (i.e., burial), and the ocean (i.e., advection).”.

Response: Added.

Line 48-50: Consider adding the underwater eddy covariance method to the list of methods for estimating aquatic metabolism. See Berg et al. 2022 (<https://doi.org/10.1146/annurev-marine-042121-012329>)

Response: Added to the list, including the citation, “...use of inert gases, and aquatic eddy covariance (Kemp and Testa 2011; Staehr et al. 2011; Berg et al. 2022).

Line 80: As written, it seems ‘assumptions’ should be singular, not plural (...can violate an assumption of the method...).

Response: Corrected.

Line 82: I appreciate that the sign of P and R estimates in the literature has been applied non-uniformly. However, I believe the convention is that P is positive (DO is produced) while R is negative (DO is consumed). Could you change the physically impossible statement to state negative P and positive R? Or add a sentence about why both values are described with a positive sign – this is somewhat described on line 236.

Response: Yes, we agree the sign has not been consistently described in the literature. We have added clarifying text at the end of the paragraph: “Note that R is often expressed as a negative value indicating consumption of dissolved oxygen. Here and throughout, we express correct values of R as positive values given the metabolic model described below.”

Line 96: Add the word statistical between ‘Bayesian’ and ‘techniques’ (i.e., Bayesian statistical techniques...)

Response: Added.

Line 98: These two cited studies – Ciavatta et al. 2008; Tassone and Bukaveckas 2019 - have used Bayesian approaches to estimate estuarine metabolism; what makes them limited? How is the approach described in this manuscript different from these two earlier studies? Have those earlier two studies informed the model selection/development described in this manuscript?

Response: Please see our response to your general comment above.

Line 106: Curious why your method builds off BASE when there has been an updated Bayesian technique for stream metabolism that more accurately estimates uncertainty and reduces equifinality - please see Appling et al. (2018) cited above. Additionally, one of the sources cited above (Tassone and Bukaveckas 2019) used the updated Bayesian technique to estimate single-station estuarine metabolism.

Response: Please see our response to your general comment above.

Line 126: Presumably, EBASE produces daily metabolic estimates. What constitutes a day in EBASE? Is it from midnight to midnight the following day or from 4 am to 4 am?

Response: The “metabolic” day in EBASE is midnight to midnight the following day. Clarifying text was added to line 182. In our experience, very similar estimates are obtained whether the day is defined midnight to midnight or some other period. This is especially true if the optimization period is greater than one day, as suggested in model application, i.e., lines 317 - 320, 523-525.

Line 129-131: I normally see water column depth represented as Z not H. Should clarify if the values of P, R, and D are positive, negative or both.

Response: The water column depth notation was changed to Z (including the documentation and code in EBASE). Clarification was added for P, R, and D on line 132: “Both P and R are expressed as positive values, whereas D can be positive (outgassing) or negative (ingassing).”

Line 135: Consider making C = Cobs if it represents the observed DO concentration. If that is not what it represents, then will need to be described in text.

Response: Yes, C represents observed dissolved oxygen concentration (as noted on line 132). We have retained C instead of using Cobs for simplicity in the model equations. Further, the addition of the model input/output table as requested by another reviewer helps clarify the input data.

Line 181: Specifying the model optimization period is an advancement of the BASE model but is not described in text. What does ‘optimization’ mean? What are the implications of using 1 day, 7 days, 30 days, or the entire time series length on the output? If you use 7 days, do you only get weekly estimates of metabolism?

Response: This was clarified in the text.

Line 181: “First, users can specify the model optimization period as the amount of time over which the unknown parameters are estimated from the Bayesian prior distributions (i.e., a, R, and b). The optimization period determines how much data are used to estimate each parameter.

Only one estimate for each of a, R, and b is returned for each optimization period as defined by the model, although P and D can vary continuously given the dependence on other inputs that can vary at each time step (e.g., PAR and wind). The optimization period can vary from a minimum of 1 day (defined as midnight to midnight the following day) to a maximum of the entire length of the time series. This differs from the BASE approach where the optimization period is set at 1 day. Sensitivity of the EBASE method to different optimization periods is described below.”

Line 185: On line 546 it is stated that linear interpolation is used, that should be described here. Furthermore, the threshold discussion on line 547-551 should be mentioned here. Lastly, on line 550-551, a 12 hour threshold should be further discussed. Why 12- hours? Why not 6 considering anything longer than 6 and you would be missing half of a semidiurnal tidal cycle.

Response: 12 hours was chosen as a default value to cover approximately half of a diurnal cycle. Users may want to consider smaller gaps if tidal cycles are having a large influence on the observed time series. Our default value was chosen under the assumption that tidal effects, although they may be present, are likely not the dominant signal in the data. If the latter is expected, detiding is strongly encouraged. We have added text to this effect.

Line 186: “All gaps are linearly interpolated to allow the model estimation to proceed continuously and any results for an optimization period with gaps larger than 12 hours are removed, eliminating the need to pre- and post-process the data when using EBASE. The user can vary the criteria for removing results (e.g., 6 hours as a more conservative criteria).”

Line 555: “More conservative gaps can be chosen if, for example, semidiurnal tidal signals operating at time scales less than 12 hours are expected to influence the results. However, detiding is strongly encouraged in these cases and the default gap size of 12 hours that describes the diurnal oxygen signal is likely appropriate after detiding.”

Also note that data for an entire optimization period are removed if any gaps greater than the chosen gap size are present, providing an additional safety measure that the results are not based on inaccurately interpolated inputs.

Line 188: With your improvements to the original BASE method, could EBASE be used to estimate metabolism in non-tidal, lotic ecosystems?

Response: In theory, EBASE could be used in non-tidal, lotic systems, since the primary difference with BASE is the use of a wind- and temperature-based gas exchange parameterization appropriate for open-water systems (Wanninkhof 2014). However, additional comparisons are needed (e.g., Odum vs EBASE in a lake) and our thorough justification for the default prior distributions are based on the estuarine literature. This is still a valuable point and we have added text to line 519:

“Further, EBASE could be applied to other non-tidal, lotic systems, although additional comparisons with existing methods are needed and the default uninformed prior distributions should be chosen carefully given the justification herein based primarily on estuarine literature (e.g., Caffrey 2004).”

Line 248-252: How was the NERRS data accessed? Also be sure to cite the NERRS system-wide monitoring program, see link on NERRS data citation here - <https://cdmo.baruch.sc.edu/data/citation.cfm>

Response: The NERRS data were accessed through the CDMO, citation was added.

Line 267: Consider rephrasing – “...has a structure similar to, yet noisier than, that of light efficiency...”.

Response: Rephrased.

Line 270-271: Wouldn't one expect the opposite? During periods of high productivity, ingassing should occur given the relatively high(er) rates of primary production. Then during periods of low productivity (i.e., outside of the growing season) that outgassing would dominate as respiration of allochthonous material continues to occur while primary production would be light limited (assuming the example dataset used is in a temperate environment).

Response: Yes, this is correct and can even be seen in Figure 2, e.g., late September to early October shows $P > R$ with negative D (ingassing), then $P < R$ with positive D (outgassing). We have corrected this error in the text.

Line 276-278: As pointed to earlier in the manuscript, it is unclear what is meant by the optimization period. Why are the results in Figure 3 averaged by the optimization period? Why not show the daily estimates? I liked seeing the fit of the EBASE estimates on the synthetic time series however, I would like to see the fit of a linear regression of the synthetic (observed) estimates vs. the EBASE (predicted) estimates.

Response: Please see the response to line 181. In particular, our revision notes that only one value each for a , R , and b is returned for each optimization period. The vertical lines for each point in Figure 3 are credible intervals showing uncertainty around each individual estimate. The statement in the caption that “the results are averaged at the time step of the model optimization period” is incorrect and removed. This really only applies to the synthetic results in Figure 5 to show a more clear comparison with the recovered values from EBASE.

Line 313: This explanation of optimization needs to come much earlier in the text and be expanded upon.

Response: Agreed, please see the response to line 181. This section was also slightly shortened in response to the changes on line 181.

Line 324-327: I'm not sure if I follow correctly - are you seeking daily metabolic estimates? If so, are the 7 & 30 day optimizations using a forward looking moving window approach that advances by one-day (similar to a rolling average)?

Response: The text was edited for clarity: “Results from optimization periods of 1, 7, and 30 days were compared to the synthetic one-year time series (b was fixed for the sensitivity analysis) based on daily averages for both the synthetic and EBASE results. For the latter, parameters that are only returned as individual values for each optimization period (a , R , and b) were assigned as daily values for comparability of summary statistics where n is the same across analyses.”

Line 473-477: It is stated that “Bayesian...methods have not been rigorously explored for estimating metabolic rates in estuaries” however, I point back to the two cited studies in the introduction (line 98) that did use Bayesian techniques to estimate estuarine metabolism. Consider rewording this sentence and/or expand on why those earlier studies are not considered rigorous.

Response: Please see our response to your general comment above. Although Tassone and Bukaveckas (2019) does provide another useful example, we still feel that these methods have not been thoroughly explored in estuaries.

Line 581: Maybe I missed it but how many MCMC simulations were used? How would a user change the number of MCMC simulations in the EBASE package? Can you provide a recommendation for the number of simulations to use or at least how many were used in this analysis?

Response: This detail was omitted and we have now included it on line 199 with the description of the MCMC approach (default 10,000 simulations).

Figures 3 & 5: These figures have a gray background while the rest are white. Please make the background color of the figures consistent across figures.

Response: Figures 3 & 5 were changed to white background.

Figure 7: Consider adding points to the lines in the left column plots. You may need to make the thickness of the lines smaller.

Response: Points were added, line thickness reduced in the left column plots.

Reviewer 2

Beck et al. developed a new method for estimating metabolism in estuaries using continuous dissolved oxygen data. Metabolism is a key component of ecosystems, yet it is inherently difficult to estimate, especially in estuaries due to tidal currents. Their method is based on a stream Bayesian approach, and the authors expanded it by adjusting the time interval over which model parameters are estimated. The longer intervals allow for estimation over tidal cycles, which acts as noise in the time series, and allows for improved model estimation. The authors also compared their model to a more conventional approach (i.e., Odum model) and show the model's improved estimation, specifically avoiding impossible results, such as negative production.

The model is written in the programming language R, making it widely available to the public. The online documentation and vignettes are clear and show the users key features and examples of the package. This is a nice bonus to go along with a well-written manuscript and expand the impact of the products.

I enjoyed reading the manuscript. It is technical where it needs to be, but also provides general context for the problem and the rationale for the technique. I was tripped up during a few of the sections, and I provide some suggestions that might improve the flow of the article. I'm also wondering if this model approach is only applicable to estuaries, or if it could be useful for other aquatic ecosystems? Overall, the authors did a great job. Nice work!

Response: Thank you for providing thoughtful comments on our manuscript. Please see our responses below.

General comments

Table of model parameters. There are several parameters, most are relatively simple (single letter), and they appear on figures. I think it would be valuable to have a table. This could include, name, acronym, units, and any other relevant information (source/equation/etc.). I can also see organizing this table by inputs and outputs (L146) to help future users identify their input data and expected outputs.

Response: We have added a new table showing model inputs/outputs, parameter names, acronyms, and units.

Is EBASE only applicable to estuaries? It seems that the main change from BASE is the inclusion of a wider temporal window to estimate model parameters and changes in the b parameterization. Can these modifications also improve upon metabolism estimates in other systems (lakes, streams, etc.)? While I see the goal of improving metabolism in estuaries, there may be wider applicability to rivers, lakes, ocean, or other coastal areas. If so, mentioning what kinds of systems (big lakes, deep lakes, big rivers, complex hydrodynamics, etc.?) would be most appropriate for the model and potential get improved estimates over other metabolism approaches. This may expand the impact of this paper.

Response: Yes, it is possible with caveats. Please see our response to reviewer one on line 188. Specifically, additional comparisons are needed and the default uninformed priors based on estuarine literature must be reconsidered.

Model parameter b.

I'm less familiar with this term, and the authors could do a little bit more to explain what it is. On L143, they say that it is "fairly well known for open for open-ocean conditions", but they never actually define the term. Looking at Eq 2, it seems to relate to "gas transfer efficiency" given that it is a coefficient on the wind-speed/viscosity term. That being said, I'm also a little confused on how Eq 3 is integrated into the model framework. Eq. 3 seems to relate more closely with streams as water depth is included as a scaler for k_w . So somehow the two models (one more typical for lentic systems, the other more typical for lotic systems) are integrated together. In theory this makes sense in an estuary as both wind and flow likely affect gas transfer.

Response: Apologies for this confusion. Eq. 3 is not used in EBASE, rather it is discussed as the gas transfer used in BASE that is inappropriate for our application, justifying use of the gas exchange model in Wanninkhof (2014). Line 166 was revised to make this more clear: "Based on this difference and the lack of availability of other possible drivers of the transfer velocity in coastal systems, Equation 3 is not used herein. Instead, the well-established wind- and temperature-based parameterization for gas exchange of Wanninkhof (2014) was used for EBASE (Equation 2)..."

Diving into eq 3, higher water levels usually indicate higher flows and thus higher gas transfer velocity (K_w). I'm not exactly sure how temperature plays into this equation, and if it is appropriate for an estuary. It seems to suggest warm periods within a day have higher exchange rates, due to differences in kinetics at the water surface. However warmer temperatures may also

reflect increased stratification and less vertical mixing (small lakes). There may be something to learn from changes in temperature that drive changes in turbulence, but simply using warmer = more exchange seems like an oversimplification. Eq 3 also includes a term related to water depth (H). In flowing waters this equation suggests that K_w increases with water level, likely a result of high-water levels = higher velocities = higher turbulence = higher k_w . In an estuary, I'm not sure this relationship truly holds as water depth is not as good of a surrogate for velocity. Highest water level may be at slack tide and thus minimal water movements. It could be that change in water depth (assuming the tidal currents are strong relative to the river inputs) would be a better term to reflect instantaneous discharge. Or possibly flow could be included as a possible input parameter. But I realize this term is not typically available.

Response: We have noted lack of clarity in our description of Equation 3 that includes the depth-dependency. As noted by Reviewer 3, Grace et al. (2015) do not include a depth-dependency in this equation. We have since revised the equation and text accordingly, emphasizing the importance of wind for the transfer velocity in open-water systems. Regarding temperature, we feel justified in its inclusion for gas exchange given the previously noted relationship with the Schmidt number, a known factor to be important in open-water systems. Also see our response to your comment on line 164.

All told, perhaps the issue with poorly constraining b is related to assumptions in the equations used to model gas exchange in an estuary. The authors do a good job explaining that the model parameter b was difficult to constrain in the example dataset. This is understandable, and my comments are mainly my mental exploration of ways that might improve that aspect of the model. I'm guessing the authors have thought extensively about this problem, and I'm mainly offering ideas. Perhaps the authors could include some other ideas for why the b parameter is difficult to constrain? Or explore additional datasets to understand when/where it can be estimated more accurately? For example, if the model was applied to an artificial dataset from a stream, lake, or other type of estuary does it perform better? If so, what is different about the system, which might help with tuning the model? Would any of these help understand the parameterization/limitation of the current model, and or identify systems it is most appropriate?

Response: Yes, we agree this issue is perplexing and worth exploring further. We have mentioned in the original draft how this could be explored further, e.g., evaluation in other locations where gas exchange may be a more dominant component of the metabolic model (line 490). We have also added a brief description of Appling et al. (2018) that confront this issue in stream metabolic models. Please see our response to the general comments from Reviewer 3.

Specific comments

L26: which open-source software? If only one (i.e., R), then can list it here.

Response: Added R in parentheses.

L40: Organic matter produced in the estuary has other outcomes. Re-respired, consumed and incorporated into biota, exported to the ocean, etc.

Response: Sentence was revised as follows: "...forming particulate organic carbon with multiple fates, e.g., buried in estuarine sediments, incorporated into biota, transferred to the ocean, etc. (Hu et al. 2006; Middelburg and Herman 2007)."

L83: which computed rates were negative? P, R, or both?

Response: Revised as “The computed rates were negative 23% of the time for both P and R...”

L128: mean depth?

Response: The software can handle a single value (e.g., mean depth) or a vector of tidal height depths equal in length to the input time series. This is expressed in the documentation: <https://fawda123.github.io/EBASE/reference/ebase.html>. This is also expressed in the new table showing model inputs/outputs as requested above.

L133: Thanks for providing the units. I am curious about area and time. I’m assuming that area is surface water area and time is the interval of the dissolved oxygen data. If so, perhaps expand on these so the author knows what the temporal and horizontal spatial scales are.

Response: Please see the new table for inputs/outputs. Although equation 1 can apply to different units of space and time, we have added those used herein in parentheses: “The equation has dimensions of moles per unit area and time (e.g., $\text{mmol m}^{-2} \text{d}^{-1}$).”

L134: “R is constant”. I believe R is allowed to vary across days, but R is constant within a day. Please specify.

Response: We have specified that the unknown metabolic parameters (a, R, and b) are constant at the unit of the model optimization period chosen by the user, although P and D vary continuously given their dependence on measured input parameters (e.g., PAR, wind) that can change at each time step. Please see our response to reviewer 1 on line 181.

L143: what is b? and for what time interval is b constant? This ends up being an output (Figure 3) and it is confusing to say that it is constant. So maybe it is constant within a day? Is this a standard parameter for gas exchange? As with the other parameters, providing some type of ‘name’ would be helpful, especially if provided in a table.

Response: Please see our response to the previous comment and the new input/output table. It’s an ambiguous parameter, but really just an indication of how sensitive the gas transfer is to wind speed. The sentence was revised as “The b parameter is fairly well known for open-ocean conditions primarily as an expression of the sensitivity of gas exchange to wind...”

L164: The equation implies that K_w would increase as water level (H) increases. It seems the authors have this statement inversed or talking about measured reaeration (K). I believe this relates to streams where increasing water levels relate to higher water velocities, and thus higher turbulence and higher gas transfer velocity (k_w). See General Comments.

Response: This was an inaccurate statement on our part. We have updated the equation and text accordingly:

Line 141: “Equation 1 is similar to the oxygen mass balance equation in BASE (Grace et al. 2015), with the main difference being the treatment of gas exchange. While both assume that gas exchange is proportional to the concentration gradient across the air–water interface, the treatments of the proportionality differ. Grace et al. (2015) used the following for the volumetric gas flux (Dvol) in BASE:

$$Dvol = [-K \cdot 1.024^{(T-\bar{T})}(C_{sat}-C)]$$

where T is the instantaneous water temperature, \bar{T} is the average water temperature over each 24-hour period in the oxygen time series (both in $^{\circ}C$), C is the measured dissolved oxygen, and C_{sat} is the saturation concentration. K is the reaeration coefficient, which was estimated from the data. In EBASE, gas flux per unit surface area of the air-water interface is proportional to the concentration gradient, with the proportionality taken from the well-established wind- and temperature-based parameterization for gas exchange of Wanninkhof (2014) (see Equation 2). EBASE also allows b to be a free parameter that may reflect spatial and temporal variability in factors other than wind and temperature that may influence transfer velocity. Wanninkhof (2014) estimated a fixed b parameter as $0.251 \text{ (cm hr}^{-1}\text{)}/(\text{m}^2 \text{ s}^{-2}\text{)}$.

L189: Thanks for putting together the web page. I'm curious if the data in this manuscript are included within the package itself, so it is possible to regenerate the results entirely? I'm also wondering how stable this website is and if any online information that is described in the manuscript will change? I'm not that familiar with these online reference materials, but I'm thinking of a static version (tag) that will stay with the paper so a reader 10 years from now could access the exact same materials that go along with this paper.

Response: It's the exception and not the norm that published software remains the same after a descriptive manuscript is published. For this reason, we have added a version of EBASE that is appropriate for this paper (v1.0.0) and included the version number in the text. EBASE is also now on CRAN, the Centralized R Archive Network, where a majority of publicly available R packages are hosted, in addition to the GitHub repository. We have also added text on line 193 indicating where source materials for this manuscript (i.e., to reproduce results) can be found: "All results provided herein were generated using the EBASE R package (specific materials for this manuscript can be found at <https://github.com/fawda123/ebase-manu>)."

L210: Thank you for providing the units for these parameters. I am wondering if that authors considered using negative exponents to ensure the division symbols are properly addressed. For example, $300 \text{ mmol/m}^2/\text{d}$. While I understand this to be $\text{mmol m}^{-2} \text{ d}^{-1}$, days could be mistakenly assumed to be in the numerator of the equation. While unlikely in this situation, the subsequent equations (L218) get even more complicated " $(\text{mmol/m}^2/\text{d})/(\text{W/m}^2)$ ", so it could be worth ensuring all the units are clear. Further, this unit has m^2 twice, so they could be removed from the final unit ($\text{mmol d}^{-1} \text{ W}^{-1}$).

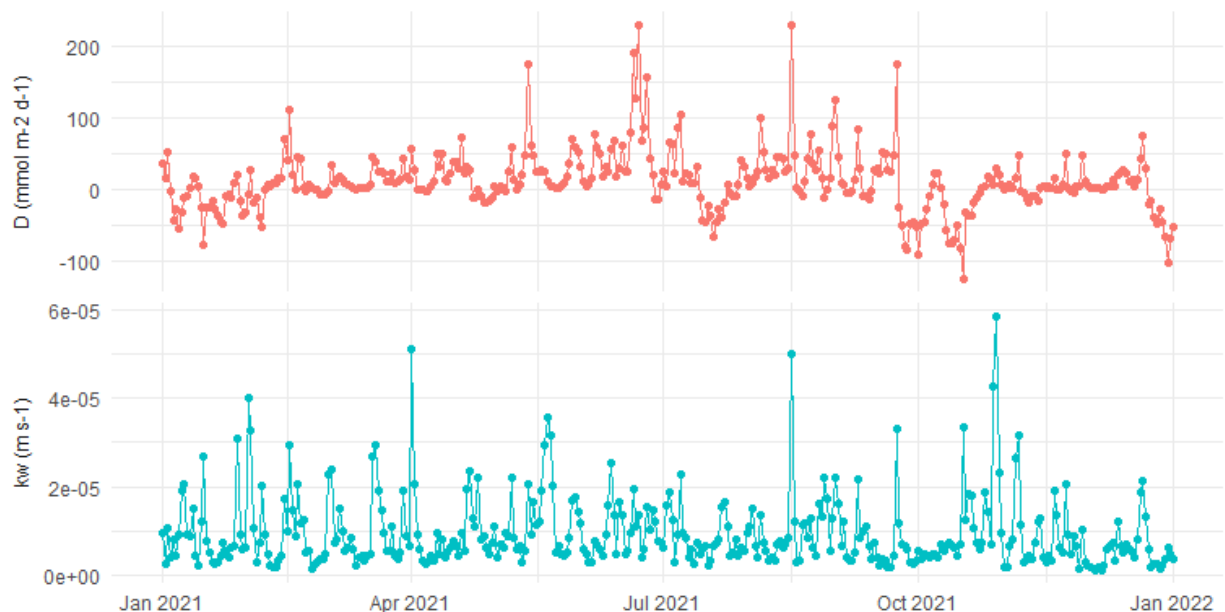
Response: Point well taken, we have not been consistent in the exponent notation as the text uses positive with fractions and the figures use negative with no fractions. We have corrected all instances in the text to use negative exponents. However, we have retained the units for a since this makes the relationship between P , a , and PAR more clear, i.e., the units for PAR (W m^{-2}) when multiplied by the units for a ($(\text{mmol m}^{-2} \text{ d}^{-1})/(\text{W m}^{-2})$) produce the units for P ($\text{mmol m}^{-2} \text{ d}^{-1}$).

L237: The upper limit of 0.502 for b . This makes sense to constrain this parameter. I also noticed that many of the estimates of b are close to this value rather than near the synthetic value for the example dataset (Figure 3). I'm wondering if anything within the model could be improved to handle this issue? See general comments.

Response: Yes, we noticed this behavior as well. To us, this is a reflection of the instability in the parameter estimation. Earlier iterations of model development did not have this constraint and the b parameter was often estimated at unreasonably high values, often causing the other parameters (a and R) to also be unreasonable. We previously described some rationale for why this parameters was so poorly constrained and offer some potential solutions for future research (i.e., lines 482-490, 502-509.)

L272: I'm curious about the model estimates for k_w . The authors show the results for flux (D), but this will vary with concentrations and k . Wondering if there is anything else to glean from those modelled results?

Response: Perhaps, although our focus was on the primary metabolic parameters returned by EBASE given the goal of assessing parameter recovery (of which k_w is included). For sake of interest, below is a plot of D and k_w for the synthetic data (data available here: https://raw.githubusercontent.com/fawda123/BASEmetab_script/master/data/apafwoxy2.csv). Note that k_w is directly proportional to wind, whereas D is mostly a function of k_w and the difference between C and C_{sat} .



L301: The units for R are listed as $(\text{mmol}/\text{m}^2/\text{d})/(\text{W}/\text{m}^2)$. Perhaps the denominator is a typo?

Response: Yes, this was a typo, corrected.

L541: Wondering if it would be helpful to mention somewhere in this paragraph, “it depends on the question/objective of the project”? For example, if we are interested in annual summations and comparisons among systems, it may be fine to use a longer optimization period. But if we are interested in daily rates, timing of events in relation to storms, floods, etc. we may need to use a shorter optimization period. So the researcher’s question should be considered.

Response: Good suggestion, we have added this text to line 541 (also note the last sentence that was added in response to a general comment from reviewer 1 regarding how frequency of continuous sampling may affect the results): “These hypotheses may relate to the length of time

over which potential factors affect metabolism, e.g., storm events may affect metabolism at short time scales and a shorter optimization period could be used, whereas longer optimization periods may be more desirable if interested in long-term, climate-related effects on metabolism. These hypotheses may also consider frequency of continuous monitoring (e.g., 15 minute vs hourly) and how this may influence the results, as this is currently unknown for EBASE.”

Reviewer 3

Beck et al. present a new software package to estimate ecosystem metabolism from time series of dissolved oxygen and accompanying physical variables in estuarine systems. Accurately estimating metabolic rates are critical to understanding impacts on estuaries and their role in material cycling. The work is highly novel as no such statistical approach is currently available for estuaries. The software adapts a package built for estimating metabolism in stream ecosystems using a Bayesian framework, which is highly suited to this task due to the ability to place prior distributions on physical parameters with known physical limitations. I found the paper to be very clear and the choices made in model development, setting of priors, and model validation to be robust and well documented. The improvements made to the model, such as the option to vary the optimization period, are valuable and were demonstrated to be important to accurately estimating rates (and mirror suggestions for dealing with inaccurate K in streams; e.g. Appling et al. 2018 <https://dx.doi.org/10.1002/2017JG004140>)

In particular, the focus on the importance of accurately capturing the physical variables is a strength of the paper. It is made clear from the outcomes of the synthetic dataset analysis that it is better to use a literature estimate of the parameter b , a constant in the equation that governs air-water exchange, then to let the model estimate inaccurate values for b . The discussion around this issue was appropriate, but I wonder if some more very clear advice could be provided to a potential user that wants to use this package to answer questions about ecosystem metabolism in estuaries but does not have the aim of further refining the modelling approaches. Could they use the estimate from Wanninkhof (2014) as was used in subsequent analyses here? Would an appropriate sensitivity analysis be to vary this estimate by 20% (as mentioned L224) to check if their P and R results are highly sensitive to this parameter? Or is further testing in a range of estuaries required before this can be applied?

Response: Thank you for these suggestions. We agree an explicit description of how the approach can be applied regarding uncertainties in the b parameter is needed. Some discussion is already included (e.g., line 488). We have also added text describing how Appling et al. (2018) addressed the issue, although this addition describes further model development rather than application. Revisions were made to the first paragraph of the discussion.

Line 490: “For application, users of EBASE may simply use a fixed value for b (e.g., $0.251 \text{ (cm hr}^{-1})/(\text{m}^2 \text{ s}^{-2})$) or perform a simple sensitivity analysis by varying b +/- a small percentage to determine how P and R may change. Further model development may consider alternative approaches for dealing with equifinality, i.e., when the same modeled DO time series can be returned with different estimates of P, R, and D. Appling et al. (2018) provide a useful example for a stream metabolic model that addresses equifinality by allowing model parameters to vary with key drivers at sub-daily scales (e.g., gas exchange versus discharge) and avoiding assumptions that model residuals are uncorrelated.”

Specific comments:

L14: The first use of “unphysical” in the abstract was a little unclear without further detail. Consider a short phrase like “may lead to estimates that are physically impossible” be used to define this first.

Response: Text was modified as suggested.

L122: The sentence “We also attempt to constrain the gas transfer velocity using this approach but are unable, at least with the data sets used in this study.” was unclear. Consider replacing “this approach” with a more precise statement (I assume “this approach” is the Bayesian framework, rather than a reference to the previous sentence on the test with the detided inputs?). I’m also not sure if “constrain” is the right word, as the issue was accurately estimating this parameter.

Response: The sentence was modified to clarify the meaning. We have retained “constrain” given that it’s used throughout the paper, but we provide an explicit meaning in parentheses: “We also attempt to constrain (i.e., accurately estimate) the gas transfer velocity using EBASE but are unable...”

L159 & L514: The air-water exchange isn’t depth dependent in BASE. The inputs (and metabolic results) in base are all volumetric and reaeration coefficient (K) is in per day. Depth is not provided to the model but can be used to convert the metabolic estimates afterwards.

Response: Thank you for pointing out this error. We have removed this from the text and revised accordingly. Please see our response to reviewer 2 for line 164.

L258: typo in “estimatd”

Response: Fixed.

L269: Should it be “availability” rather than “variability”? of course, a more variable pool of organic matter could also be correct.

Response: Changed to “availability”, this seems more correct.

L352: The “right answer for wrong reasons” is interesting. It could be clearer here that even though DO is estimated accurately, the P and R estimates will be inaccurate in this scenario.

Response: Sentence was revised as follows: “...the potential for the model to produce the right answer (accurate DO) for the wrong reasons (inaccurate P, R, or D), since DO is simply a mass balance of P, R, and D (Equation 1). This issue, or equifinality, has been encountered in stream metabolic models (Appling et al. 2018).”

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**Fitting metabolic models to dissolved oxygen data: The
Estuarine BAYesian Single-station Estimation method
(EBASE)**

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Running head: EBASE metabolic model

Key words: Bayesian, dissolved oxygen, ecosystem metabolism, estuary, gas exchange, open-source

Abstract

Continuous measurements of dissolved oxygen (DO) are useful for quantifying ecosystem metabolism, which is critical for understanding estuarine biogeochemistry and ecology, but current methods applied to these data may lead to estimates that are physically impossible and poorly constrained errors. Here we present a new approach for estimating estuarine metabolism: EBASE (Estuarine BAYesian Single-station Estimation). EBASE applies a Bayesian framework to a simple process-based model and DO observations, allowing the estimation of critical model parameters, specifically light efficiency and respiration, as informed by a set of prior distributions. EBASE improves upon the stream-based model from which it was derived by accommodating missing DO data and allowing the user to set the time period over which parameters are estimated. We demonstrate that EBASE can recover known metabolic parameters from a synthetic time series, even in the presence of noise (e.g., due to tidal advection) and when

prior distributions are uninformed. Optimization periods of 7 days and 30 days are more preferable than 1 day. A comparison with the more-conventional method of Odum reveals the ability of EBASE to avoid unphysical results (such as negative photosynthesis and respiration) and improves when the DO data are detided. EBASE is available using open-source software (R) and can be readily applied to multiple years of long-term monitoring data that are available in many estuaries. Overall, EBASE provides an accessible method to parameterize a simple metabolic model appropriate for estuarine systems and will provide additional understanding of processes that influence ecosystem status and condition.

Introduction

Estuaries play a key role in the global cycling of elements because of high rates of biogeochemical activity at the interface between land, river, ocean, and atmosphere. As materials are transported from land to rivers to ocean, estuaries profoundly transform or filter these materials through various processes, chief among which are primary production and respiration, collectively referred to as metabolism (Schubel and Kennedy 1984). For example, estuarine respiration of organic carbon delivered from land produces carbon dioxide, which may be lost to the atmosphere via outgassing (e.g., Cai 2011). Similarly, estuarine primary production consumes dissolved inorganic carbon delivered from land, forming particulate organic carbon with multiple fates, e.g., buried in estuarine sediments, incorporated into biota, transferred to the ocean, etc. (Hu et al. 2006; Middelburg and Herman 2007). Estuarine metabolic processes are fundamentally important, as illustrated by the dissolved inorganic carbon budget of eastern North American estuaries (Najjar et al. 2018); net primary production and heterotrophic respiration far exceed inputs from upland sources and outputs to the atmosphere and ocean. As such, small changes in either net primary production or heterotrophic respiration can have a large impact on

the difference between the two, net ecosystem metabolism (NEM, sometimes also referred to as net ecosystem production), which ultimately governs the form and quantity of estuarine materials that are lost to the atmosphere (i.e., outgassing), the sediments (i.e., burial), and the ocean (i.e., advection).

Methods for estimating metabolism in aquatic environments are numerous and include open-water techniques, bottle-based incubations, ecosystem budgets, oxygen isotopes, use of inert gases, and aquatic eddy covariance (Kemp and Testa 2011; Staehr et al. 2011; Berg et al. 2022).

Based on the variety of assumptions and limitations of each method, comparisons of metabolic rates within and between ecosystems have been challenging. For example, an assessment in Randers Fjord (Denmark) showed agreement in both the sign and magnitude among four different approaches (Gazeau et al. 2005). However, gross primary production and ecosystem respiration estimates from incubations were consistently lower than those from open-water methods, consistent with the estuarine respiration synthesis of Hopkins and Smith (2005).

Even within one technique, there are numerous choices to be made that alter the outcome. For example, in the commonly used ^{14}C technique for measuring primary production, Cloern et al. (2014) noted that investigators have made divergent choices with regard to filtering mesozooplankton grazers, measuring ^{14}C in dissolved organic carbon, changing spectral light quality with depth, the euphotic zone depth, the incubation time, and the incubation location (*in situ* vs. on-deck). These challenges are further compounded in estuaries, where high temporal and spatial variability have been noted in global syntheses of photosynthesis and respiration. Cloern et al. (2014) found that annual phytoplankton primary production can vary 10-fold within an estuary and up to 5-fold from year to year. Hopkins and Smith (2005) focused on cross-system variations and found benthic and pelagic respiration rates varying by more than factors of

30 and 40, respectively, ranges that are broadly consistent with whole-system respiration rates based on the open-water method (Hoellein et al. 2013).

Advances in sensor technology for continuous collection of dissolved oxygen time series suggest that the open-water method (Odum 1956) could be leveraged for applications across multiple locations. This method exploits the diel cycle of dissolved oxygen and allows the simultaneous determination of whole-system gross primary production ($P = \text{net primary production} + \text{autotrophic respiration}$), ecosystem respiration ($R = \text{heterotrophic} + \text{autotrophic respiration}$), and NEM ($P - R$). A global synthesis of warm-season, open-water metabolism studies (Hoellein et al. 2013) was based on a total of 47 estimates, almost all of which were derived from a single study of U.S. estuaries (Caffrey 2004). A similar synthesis was done by Yvon-Durocher et al. (2012). These studies evaluated the open-water method as applied to continuous monitoring data available for several decades across the National Estuarine Research Reserve System (NERRS), a network of 30 estuaries across the U.S. Thus, the approach can be broadly applied where data are available, although it is not without limitations. In particular, tidal advection can violate an assumption of the method that the measurements are from the same parcel of water with a continuous metabolic history (Kemp and Boynton 1980). Striking evidence of this limitation is the large number of physically impossible negative P and R estimates in the open-water analysis of 28 3-year time series by (Caffrey 2003). The computed rates were negative 23% of the time for both P and R , on average, and as high as 69% for individual sites. Note that R is often expressed as a negative value indicating consumption of dissolved oxygen. Here and throughout, we express correct values of R as positive values given the metabolic model described below.

91 Another limitation of the open-water method is the estimation of the air–water oxygen flux,
92 which is an important term in the oxygen budget. Most approaches estimate this flux using an
93 empirically derived gas transfer velocity that is dependent on wind speed and temperature or held
94 at a constant value (e.g., Caffrey 2004; Russell and Montagna 2007; Nagel et al. 2009; Beck et
95 al. 2015; Murrell et al. 2018). Particularly challenging is that the exchange velocity in estuaries
96 also depends on water depth and tides (Ho et al. 2016) and possibly additional factors, such as
97 fetch and the concentration of total suspended solids (Borges and Abril 2011). The importance of
98 the air–water gas flux in the oxygen budget opens up the possibility that the oxygen data
99 themselves may be used to determine the gas transfer velocity, an approach that has been applied
100 in streams (e.g., Riley and Dodds 2013).

101 A unified model to explain the large variability of metabolic rates within and across estuaries is
102 clearly lacking as a critical tool for understanding metabolic processes. Bayesian statistical
103 techniques have only been explored in limited estuarine applications despite their potential to
104 address the above (e.g., Tassone and Bukaveckas 2019). Bayesian models allow for
105 incorporation of prior knowledge about model parameters and robust estimation of parameter
106 probability distributions (Holtgrieve et al. 2010) using highly efficient computational algorithms
107 (Grace et al. 2015; Winslow et al. 2016). These techniques are very powerful because they not
108 only estimate P and R as standard open-water methods do, but they retrieve estimates and their
109 uncertainties of parameters related to gas exchange, P, and R (e.g., the initial slope of the
110 photosynthesis–irradiance curve), which reveals quantitative information about the mechanisms
111 of metabolism and gas exchange. Tassone and Bukaveckas (2019) adapted a Bayesian approach
112 developed for streams (Appling et al. 2018) in an estuarine setting to estimate metabolic rates in
113 the James River. Although this approach demonstrated the utility of such an approach in

estuaries, much of the core model structure developed for streams was unchanged and may not have been fully descriptive of fundamental processes influencing metabolism in open-water environments. Another potentially useful application developed for streams is the Bayesian Single-station Estimation (BASE) method (Grace et al. 2015). BASE has been demonstrated to accurately determine metabolic parameters and their uncertainty using continuous monitoring data that are similar to those available at many estuarine locations. The underlying model components can also easily be updated given the relatively simple format of the approach. As such, modification of BASE to include model characterizations more appropriate for estuaries, while maintaining the fundamental Bayesian approach, could prove useful.

The goal of this paper is to describe the development and application of a new Bayesian method for simultaneously determining gross primary production and ecosystem respiration in estuaries from high-resolution dissolved oxygen time series. We call this method EBASE (Estuarine Bayesian Single-station Estimation), which builds and improves on the BASE method (Grace et al. 2015) using an approach more appropriate for estuarine time series. We focus on BASE given the relative simplicity and, therefore, ease of application compared to other stream-based Bayesian approaches (e.g., Appling et al. 2018). The rationale and changes made to BASE are described in detail, followed by a demonstration of how EBASE can estimate known metabolic parameters with reasonable certainty from a synthetic time series. Lastly, metabolic estimates from EBASE are compared with those of the Odum open-water method to identify key differences related to both the theoretical and statistical differences associated with each method. These comparisons combine results using real observations and those based on detided dissolved oxygen inputs to demonstrate effects of tidal advection on metabolic estimates. We also attempt to constrain (i.e., accurately estimate) the gas transfer velocity using EBASE but are unable, at

least with the data sets used in this study. EBASE is available as an open-source software package created with the R statistical programming language (<https://cran.r-project.org/web/packages/EBASE/index.html>, Beck et al. 2024; R Core Team 2023) and the results herein provide practical suggestions for use of the software on novel datasets.

Materials and Procedures

EBASE uses a mass balance equation for dissolved oxygen, assuming a well-mixed water column of depth Z and no lateral transport processes:

$$Z \frac{dC}{dt} = P - R + D \quad (1)$$

where the terms on the right side of the equation are gross primary production (P), ecosystem respiration (R), and the net upward diffusive gas flux at the air–water interface (D), respectively, processes that result in the change in dissolved oxygen concentration (dC) per unit time (dt). Both P and R are expressed as positive values, whereas D can be positive (ingassing) or negative (outgassing). The equation has dimensions of moles per unit area and time (e.g., $\text{mmol m}^{-2} \text{d}^{-1}$). P is modeled as $aPAR$, where PAR is the surface photosynthetically active radiation and a is the light efficiency; R is constant; and D is modeled in the standard manner (e.g, Sarmiento and Gruber 2013) as $k_w(C_{sat} - C)$, where k_w is the gas transfer velocity and C_{sat} is the saturation (or equilibrium) concentration, calculated from salinity and temperature (García and Gordon 1992). The gas transfer velocity is modeled using the formulation in Wanninkhof (2014):

$$k_w = bU_{10}^2 \left(\frac{Sc}{600} \right)^{-0.5} \quad (2)$$

where b is constant, U_{10} is the wind speed at 10 m above the water, and Sc is the Schmidt number, which is the ratio of the kinematic viscosity of water to the molecular diffusivity of oxygen in water (Sc is computed from water temperature and salinity using the polynomial fit in Wanninkhof 2014). The b parameter is fairly well known for open-ocean conditions primarily as an expression of the sensitivity of gas exchange to wind, but may be different in estuaries, where the transfer velocity is influenced by factors other than wind speed and Sc . As such, the three parameters estimated by EBASE are a , R , and b using the required input data that include time series of dissolved oxygen, water temperature, salinity, PAR, wind speed, and water column depth (Table 1).

Changes to BASE

Equation 1 is similar to the oxygen mass balance equation in BASE (Grace et al. 2015), with the main difference being the treatment of gas exchange. While both assume that gas exchange is proportional to the concentration gradient across the air–water interface, the treatments of the proportionality differ. Grace et al. (2015) used the following for the volumetric gas flux ($Dvol$) in BASE:

$$Dvol = [K \cdot 1.024^{(T - \bar{T})}(C_{sat} - C)] \quad (3)$$

where T is the instantaneous water temperature, \bar{T} is the average water temperature over each 24-hour period in the oxygen time series (both in °C), C is the measured dissolved oxygen, and C_{sat} is the saturation concentration. K is the reaeration coefficient, which was estimated from the data. In EBASE, gas flux per unit surface area of the air–water interface is proportional to the concentration gradient, with the proportionality taken from the well-established wind- and temperature-based parameterization for gas exchange of Wanninkhof (2014) (see Equation 2).

EBASE also allows b to be a free parameter that may reflect spatial and temporal variability in factors other than wind and temperature that may influence transfer velocity. Wanninkhof (2014) estimated a fixed b parameter as $0.251 \text{ (cm hr}^{-1}\text{)}/(\text{m}^2 \text{ s}^{-2})$.

BASE was also modified by removing the temperature dependence of respiration and the potential for P to depend nonlinearly on PAR. While there is evidence for both dependencies in aquatic systems, we found, in preliminary model runs, that model stability was enhanced when these dependencies were removed. It would be straightforward to include such dependencies in EBASE as our understanding of them improve and as data become available that will allow them to be robustly constrained.

For ease of application, an R package was developed to implement EBASE (<https://cran.r-project.org/web/packages/EBASE/index.html>, Beck et al. 2024; R Core Team 2023), similar to the R package available for BASE (<https://github.com/dgiling/BASEmetab>). EBASE differs from BASE in model implementation in two ways. First, users can specify the model optimization period as the amount of time over which the unknown parameters are estimated from the Bayesian prior distributions (i.e., a , R , and b). The optimization period determines how much data are used to estimate each parameter. Only one estimate for each of a , R , and b is returned for each optimization period as defined by the model, although P and D can vary continuously given the dependence on other inputs that can vary at each time step (e.g., PAR and wind). The optimization period can vary from a minimum of 1 day (defined as midnight to midnight the following day) to a maximum of the entire length of the time series. This differs from the BASE approach where the optimization period is set at 1 day. Sensitivity of the EBASE method to different optimization periods is described below. Second, the EBASE software can accommodate missing observations in the input data by interpolating gaps prior to estimating the

metabolic parameters. All gaps are linearly interpolated to allow the model estimation to proceed continuously and any results for an optimization period with gaps larger than 12 hours are removed, eliminating the need to pre- and post-process the data when using EBASE. The user can vary the criteria for removing results (e.g., 6 hours as a more conservative criteria). Again, this feature was not included in the original BASE method and a complete time series was required for use. A detailed web page (<https://fawda123.github.io/EBASE/>) describes how to use the package, with explanations of the functions for viewing model results, including a plot of the modeled dissolved oxygen with the observed, a time series plot of the oxygen budget terms (P , R , and D), and a time series plot of the credible intervals for the a , R , and b parameters. All results provided herein were generated using the EBASE R package (v1.0.1, specific materials for this manuscript can be found at <https://github.com/fawda123/ebase-manu>).

EBASE model estimation

The parameters a , R , and b are estimated by likelihood given the observed data and prior distributions for the parameters. The “Just Another Gibbs Sampler” (JAGS) software (as for BASE, Plummer et al. 2003) is used with the EBASE R package (described above) to estimate probability distributions of the unknown parameters using Markov Chain Monte Carlo (MCMC) simulations (default 10,000) in a Bayesian framework applied to a finite-difference form of Equation 1. A JAGS model file is included with the package that implements Equation 1, with options to supply a custom model file as needed. All parameter inputs and outputs for EBASE are shown in Table 1.

The metabolism estimates and their parameters returned by the Bayesian routine implemented in JAGS are affected by the prior distributions assigned to each. As for BASE, relatively uninformed prior distributions following a normal Gaussian distribution are used by default,

although the priors can be changed based on previous knowledge of parameters specific to an ecosystem or as informed by other metabolic modeling approaches. Reasonable uninformed prior distributions for EBASE were chosen with mean values using approximate estimates from the literature (Caffrey 2004; Wanninkhof 2014) and standard deviations that were sufficiently large to allow the Bayesian routine to search an unconstrained parameter space.

Specifically, the prior mean for R was chosen as $300 \text{ mmol m}^{-2} \text{ d}^{-1}$ ($\sim 10 \text{ g O}_2 \text{ m}^{-2} \text{ d}^{-1}$) using a synthesis based on NERRS data (Table 2 in Caffrey 2004). Although this synthesis focused on small, shallow estuaries that are part of the NERRS, this dataset is the largest, longest, and most consistently collected in the US and it is reasonable to expect others may apply EBASE to these data. The prior mean for a was chosen assuming that P and R are comparable at long time scales, such that $aPAR = R$, or $a = (300 \text{ mmol m}^{-2} \text{ d}^{-1})/PAR$. Using the global mean surface PAR of 80 W m^{-2} , which is based on a global mean surface total shortwave radiation of 200 W m^{-2} (Kiehl and Trenberth 1997) and a PAR fraction of total shortwave radiation of 0.4 (Jacovides et al. 2004), the prior mean for a is reasonably set at $4 \text{ (mmol m}^{-2} \text{ d}^{-1})/(\text{W m}^{-2})$. Lastly, the prior mean for b was chosen as $0.251 \text{ (cm hr}^{-1})/(\text{m}^2 \text{ s}^{-2})$ following Wanninkhof (2014).

The prior standard deviation for R was based on the standard deviation of the mean values of R at the NERRS sites in Caffrey (2004). The standard deviation of R was $171 \text{ mmol m}^{-2} \text{ d}^{-1}$, which was rounded to 50% of the mean, or $150 \text{ mmol m}^{-2} \text{ d}^{-1}$. The standard deviation for a was set proportionally to $2 \text{ (mmol m}^{-2} \text{ d}^{-1})/(\text{W m}^{-2})$. For the prior standard deviation of b , we considered using the 20% error estimated for b by Wanninkhof (2014). However, we chose a larger value, 50%, because the wind speed-based gas transfer velocity formulation of Wanninkhof (2014) was mainly developed and calibrated for open-ocean applications, where the

complications of surfactants (Frew 1997) and tidal currents (Ho et al. 2016), as well as fetch and suspended matter (Borges and Abril 2011), are expected to be minimal.

Together, the default prior distributions for a , R , and b (Figure 1) are:

$$a \sim N(4,2)I(0,\infty) \text{ (mmol m}^{-2} \text{ d}^{-1})/(\text{W m}^{-2}) \quad (4)$$

$$R \sim N(300,150)I(0,\infty) \text{ mmol m}^{-2} \text{ d}^{-1} \quad (5)$$

$$b \sim N(0.251,0.125)I(0,0.502) \text{ (cm hr}^{-1})/(\text{m}^2 \text{ s}^{-2}) \quad (6)$$

where $N(\alpha,\beta)$ indicates a normal distribution with mean α and standard deviation β and $I(\gamma,\theta)$ is 1 between γ and θ and 0 elsewhere; I has the effect of truncating the normal distribution to minimum and maximum values. All prior distributions were constrained to positive values based on known physical constraints and requirements of the model formula in Equation 1.

Additionally, the prior distribution for b was constrained to an upper limit of 0.502 (cm hr⁻¹)/(m² s⁻²) (~twice the default mean). Initial development of EBASE showed that using an undefined upper limit of b led to unstable and unreasonable estimates for all parameters. Functions in the EBASE R package allow alternative prior distributions from those above.

Assessment

EBASE comparison with known results

A preliminary assessment of the ability of EBASE to produce reasonable parameter estimates for a , R , and b (Equation 1) was conducted using a synthetic time series of dissolved oxygen concentration created from observed water temperature, salinity, air temperature, PAR , and wind speed measured every 15 minutes. This assessment evaluated if (1) EBASE estimates similar values for the known parameters used to create the synthetic time series, and (2) how the

estimated values change with different model configurations. The synthetic time series used inputs from one year (2021) of continuous data from the NERRS reserve in Apalachicola Bay, Florida (NOAA NERRS 2023). Water temperature and salinity were from the Cat Point water quality monitoring station (29.7021 ° N, 84.8802 ° W) and the meteorological observations were from the nearby East Bay station (29.7694 ° N, 84.8815 ° W, ~10 km north of Cat Point). Missing observations in the water and meteorological data (5.1% and 3.4% of all observations in each dataset, respectively) were filled using autoregressive modelling (Akaike 1969) of the actual data versus time to create a complete dataset from January 1st to December 31st.

The synthetic oxygen time series was generated using Equation 1 as a forward calculating model with specified daily values for a , R , and b . The b parameter was fixed at $0.251 \text{ (cm hr}^{-1}\text{) / (m}^2 \text{ s}^{-2}\text{)}$ (Wanninkhof 2014). Daily values of a and R were estimated by (1) applying the Odum open-water method as implemented in the WtRegDO R package (Beck 2023), (2) computing monthly averages of the resulting daily estimates of P and R , (3) computing the monthly average of the parameter a by dividing the monthly average of P by the monthly average of PAR , and (4) by fitting a spline function to the monthly averages of R and a .

The resulting synthetic time series of light efficiency, dissolved oxygen budget terms (P , D , and R), and dissolved oxygen concentration are shown in Figure 2. The light efficiency has a complex structure, with maxima in the summer, fall, and winter, and a strong minimum in spring (Figure 2a). The oxygen budget terms (Figure 2b) reveal that (1) photosynthesis has a structure similar to, yet noisier than, that of light efficiency, reflecting the synoptic-scale variability of PAR ; (2) respiration has the expected structure of being greatest during the summer (Caffrey 2004), stimulated by greater autochthonous organic matter availability and high temperature; and (3) the air–water gas flux mimic productivity on short time scales, with outgassing during high

productivity and ingassing during low productivity. The synthetic dissolved oxygen time series shows high variability at multiple time scales (Figure 2c). There is a prominent diurnal cycle that is superimposed on subseasonal variability, presumably driven by radiation and winds.

Recovery of model parameters

The synthetic time series was used as input to EBASE to predict metabolic parameters with the default prior distributions above. Two optimization periods of 7 and 30 days were evaluated. This analysis provided a demonstration that the default priors are not entirely unreasonable based on the ability to reproduce the known parameters in the synthetic time series (Figure 3). Overall, EBASE produced reasonable results for a and R , with higher accuracy using the 30 day optimization period (Figure 3b) compared to the 7 day optimization period (Figure 3a). However, the model was unable to return the b parameter with acceptable accuracy, suggesting the data were insufficient to constrain this parameter. Further, many of the 95% credible intervals from the posterior distributions of each parameter did not overlap the known values from the synthetic time series. Estimates for each optimization period may be inaccurate despite overall similarities comparing all estimates to the known values for the whole year.

Sensitivity to priors

Several configurations of the EBASE model can influence how the parameters and metabolic rates are estimated. Two types of sensitivity analyses were conducted to evaluate changes in the results returned by EBASE, where in all cases, the results were compared to the known values in the synthetic time series. First, results were compared to the known values after changing characteristics of their prior distributions. Second, results were compared using a model period of optimization for 1, 7, and 30 days to assess how results varied based on the amount of data used for the Bayesian estimation. Details of these analyses are as follows.

313 The prior distributions for the EBASE parameters follow truncated normal distributions with
314 defined means (μ) and standard deviations (σ) (Equations 4, 5, and 6). The sensitivity analysis
315 evaluated changes in the distributions by varying the means and standard deviations from small
316 to large to test the effect of changes in the central tendencies and more or less constrained ranges,
317 respectively, on the results. Low and high values for the means and standard deviations for R
318 were assessed following reasonable ranges from Caffrey (2004) using logic similar to that for
319 choosing the default priors. The minimum and maximum mean values for R were evaluated as
320 138 and 1009 $\text{mmol m}^{-2} \text{d}^{-1}$, which we rounded to 1/2 and 3 times the mean (150 and 900
321 $\text{mmol m}^{-2} \text{d}^{-1}$) and proportionally for a as 2.0 and 12 ($\text{mmol m}^{-2} \text{d}^{-1})/(\text{W m}^{-2})$. The
322 minimum and maximum values for the standard deviations for R and a were chosen as 10% and
323 1000% of the default mean values to test a range from high precision to completely uninformed
324 values. The mean and standard deviation for the b parameter were not tested and the prior value
325 was set as the fixed constant used in the synthetic time series, $0.251 (\text{cm hr}^{-1})/(\text{m}^2 \text{s}^{-2})$. There
326 is minimal prior knowledge on expectations for the b parameter and initial assessments with the
327 synthetic time series demonstrated that the parameter was poorly constrained, primarily because
328 the fixed parameter could not be estimated using observed data (i.e., wind, water temperature)
329 that affected the actual realization of b . As such, each unique combination of low and high
330 values for the means and standard deviations for a and R were evaluated, creating $2^4 = 16$
331 different combinations of prior distributions that were used with the synthetic time series in
332 EBASE.

333 The optimization period used for a time series determines how much data are used to estimate
334 the metabolic parameters. A short period of optimization (e.g., 1 day) may return unstable
335 parameter estimates if forcing factors (e.g., wind, temperature) that affect estuarine

biogeochemical rates occur at time scales longer than the chosen period of optimization for EBASE. As such, potentially longer optimization periods may return more stable and robust estimates given that more data are used for parameter estimation, although at the risk of overgeneralizing metabolic rates if biogeochemical variation occurs at time scales less than the optimization period. Results from optimization periods of 1, 7, and 30 days were compared to the synthetic one-year time series (b was fixed for the sensitivity analysis) based on daily averages for both the synthetic and EBASE results. For the latter, parameters that are only returned as individual values for each optimization period (a , R , and b) were assigned as daily values for comparability of summary statistics where n is the same across analyses. For the models with 7 and 30 day optimization periods, the final period in the annual time series was excluded from the results due to incomplete number of observations compared to earlier periods (i.e., the total number of days in the time series was not evenly divided by 7 or 30, resulting in a remainder for the last period). Each optimization period was also evaluated for every unique combination of prior distributions, totaling 48 (16 times three optimization periods) unique analyses for the assessment of changing priors of all parameters.

Changing the prior distributions affected the ability of EBASE to return the known parameters from the synthetic time series, with results varying by optimization period. [Figure 4](#) shows a summary of the comparisons of the synthetic data with EBASE for each unique combination of prior distributions and the three optimization periods of 1, 7, and 30 days. The results are shown using Nash-Sutcliffe Efficiency (NSE) values (Nash and Sutcliffe 1970; Moriasi et al. 2007):

$$NSE = 1 - \frac{\sum_{i=1}^n (Y_i^{Syn} - Y_i^{EBASE})^2}{\sum_{i=1}^n (Y_i^{Syn} - \bar{Y}^{Syn})^2} \quad (7)$$

where Y_i is the estimate from EBASE or the synthetic times series for the optimization period i , evaluated for each of five model outputs (D , DO , R , a , and P), each of 16 unique combinations of priors, and each of 3 optimization periods. The value n is the number of optimization periods in the one-year time series, i.e., $n = 365$ for comparability among the optimization periods. The NSE value is conceptually similar to the coefficient of determination, but varies from $-\infty$ to 1. Values in the positive range from 0 to 1 are desirable with 1 being a perfect fit, whereas values in the negative range indicate the mean of the synthetic data is a better predictor than EBASE.

Several conclusions can be made from the results in Figure 4 following the patterns of the NSE values. Overall, most models regardless of optimization period or priors were able to show some skill at reproducing the dissolved oxygen time series, which had a median NSE across all optimization periods and priors of 0.91. The only models where the NSE values were less than zero for dissolved oxygen were those where σ of the a and R parameters was low and μ for one of the a and R parameters was high. However, substantial variation in NSE values was observed among all other model outputs, with some very low values of NSE occurring while the DO simulation was fairly good, showing the potential for the model to produce the right answer (accurate DO) for the wrong reasons (inaccurate P , R , or D), since DO is simply a mass balance of P , R , and D (Equation 1). This issue, or equifinality, has been encountered in stream metabolic models (Appling et al. 2018). After dissolved oxygen, gas exchange (D) was estimated with the highest median NSE of 0.73. This result makes sense, given that differences in D across all optimization periods and priors are due solely to difference in DO . Conversely, the a parameter was reproduced the most poorly, with a median NSE of -0.75.

By optimization period, median NSE values across all model outputs increased as the number of days used for model optimization increased (1 day = -2.42, 7 days = 0.26, 30 days = 0.6). The

top three ranked models were identical for the 1 and 7 day optimization period, whereas the top three models for the 30 day optimization appeared less dependent on the choice of priors. Median NSE values across model outputs for the top models increased with optimization period (1 day = 0.09, 7 days = 0.44, 30 days = 0.64). The NSE values for all model outputs were greater than zero for the top three models in the 30 day optimization period, whereas the a parameter had NSE less than zero for the top model in the 7 day optimization period and R and a had negative NSE values for the top model in the 1 day optimization period. Less than half of the model outputs regardless of optimization period or priors had $\text{NSE} < 0$ (43%). As such, the prior combinations that produced the highest NSE values across all parameters were those where all prior distributions had low μ and σ values for both a and R for the 1 and 7 day optimization periods, whereas the combination of priors did not have a notable effect on the output for the 30 day optimization period. Notably, many of the top models for the shorter optimization periods had at least one high value for σ for a or R , suggesting that models with sufficient flexibility to search a larger parameter space can produce metabolic estimates most similar to actual values. The actual model results for the best and worst performing combinations of prior distributions for the three optimization periods are shown in Figure 5 (all results are averaged at the time-step of the optimization period for visual comparability). The best performing models were those with the highest median NSE values across all model outputs in Figure 4. The best performing models for each optimization period (Figure 5 a, c, e) showed similar results where the model outputs were similar to the synthetic time series, although more variation in the EBASE results were of course observed with the 1 day optimization period. The worst performing models for the 1 and 7 day optimization periods (Figure 5 b, d) demonstrate the negative NSE values that were obtained (i.e., EBASE values much lower or higher than the synthetic values). The worst

performing models were caused by constraining EBASE to a small parameter space, such as a high μ and low σ for a as in the bottom row for subplots (b) and (d). In such cases, the *DO* simulation (fourth row) can still be quite good as a result of compensating errors in a and R . The EBASE-derived rates of photosynthesis and respiration are both much higher than in the synthetic data for subplots (b) and (d), errors that compensate well enough to produce fairly accurate recoveries of the *DO* time series. Further, results for the worst model for the 30 day optimization period in subplot (f) are visually indistinguishable from those of the best model in subplot (e), suggesting that poor estimates from inadequate priors can in part be mitigated using longer optimization periods.

Impact of noise on parameter recovery

As a final evaluation of EBASE to return known metabolic parameters, a second synthetic time series was created that added estimated effects of noise to the original synthetic time series. The objective of the analysis is to develop an expectation of how metabolic estimates may change using *in situ* data with noise that may substantially mask a biological signal in dissolved oxygen measurements. The noise estimates were created using a weighted regression analysis (Beck et al. 2015; Beck 2023) on observed dissolved oxygen time series for Apalachicola Bay in 2021. This approach models dissolved oxygen as a function of time (day), hour, and water depth using a moving window approach with weights of the independent variables appropriate for each time period within the windows. The results of this analysis return a predicted and detided dissolved oxygen time series, where the detided results are simply the predictions at average tidal height (see Beck et al. 2015 for details). This method was only applied to dissolved oxygen since it has not been evaluated with any other parameters. Two separate time series of noise, representing residual (any other random process not related to metabolism or tidal advection) or tidal noise,

were derived from the observed, predicted and detided time series. The residual noise was estimated as the difference between the observed and predicted time series and the tidal noise was estimated as the difference between the predicted and detided time series (Figure 6a). Both the residual and tidal noise were added to the original synthetic time series in Figure 2c and are shown in Figure 6b. EBASE was then used on the synthetic time series with noise, then compared with results from the original synthetic time series. The default priors (Equations 4 and 5) were used with a 7 day optimization period. The prior for the b parameter was fixed at $0.251 \text{ (cm hr}^{-1}\text{)}/(\text{m}^2 \text{ s}^{-2})$ following similar logic used for the sensitivity analysis described above. Figure 7 shows the comparison of the results recovered from EBASE for the synthetic time series with noise (residual and tidal) and for the synthetic time series without noise. EBASE was able to recover reasonable estimates for both a and R , although the results from the noisy time series were slightly biased towards higher values as shown by the blue regression lines on the right side of Figure 7. The higher values for a will produce higher estimates for P , and combined with R , will produce inflated values for metabolic estimates compared to the results for the synthetic time series without noise. Although the results for the latter were not biased towards higher values, both estimates provided by EBASE had a relatively large range of variability around the known values. As noted above, a longer optimization period could reduce this variability.

EBASE and Odum comparison with real observations

Metabolic estimates from EBASE were further compared to those from existing methods to benchmark and evaluate potential differences from alternative model formulations used by each approach. The observed one-year continuous time series described above for water quality and weather data from Apalachicola Bay was used to compare metabolic estimates from EBASE and

the Odum open-water method (Odum 1956). The Odum method used an approach described in Murrell et al. (2018) created for estuarine application that uses a gas-exchange approach from Thébault et al. (2008). For a better comparison with the EBASE methods, the gas exchange parameterization in the Odum method was modified to use the Wanninkhof (2014) approach and the b parameter was fixed at $0.251 \text{ (cm hr}^{-1})/(\text{m}^2 \text{ s}^{-2})$ (as available in the WtRegDO R package, Beck 2023). An additional and fundamental difference between EBASE and the Odum method is that the former is likelihood-based with metabolic rates estimated by fitting the model to the data, whereas the latter is strictly arithmetic-based primarily on integration of the diel dissolved oxygen curve. Thus, potentially different results are expected based on the alternative statistical approaches to estimate the metabolic results. Each comparison also evaluated differences in the results using the observed dissolved oxygen time series and a detided time series using weighted regression (Beck et al. 2015; Beck 2023). The latter comparison provided an assessment of metabolic rates that are expected to be minimally influenced by tidal advection, as a fundamental assumption of metabolic models using *in situ* dissolved oxygen time series from fixed monitoring stations. The prior distributions for EBASE used the default values (Equations 4, 5, and 6). Similar to the previous analyses, the prior distribution for the b parameter was fixed given the difficulty in recovery. A 1 day model optimization period was used for EBASE for comparability with the Odum method that returns daily estimates.

Pairwise comparisons of the daily estimates of NEM , P , and R returned by each method were evaluated using simple summary statistics, including Pearson correlation coefficients (ρ) and root mean square differences (RMSD) of the linear regression fit comparing the same flux type between methods. Figure 8 and Table 2 provide a comparison of the metabolic estimates from the EBASE and Odum methods. Correlations for all metabolic estimates, regardless of the input

time series, were positive and significantly correlated, as expected. However, correlations were generally stronger (and RMSDs smaller) for the metabolic results based on the detided dissolved oxygen time series. The observed time series clearly produced a much larger range of values for results from both the EBASE and Odum methods.

The comparisons in [Figure 8](#) and [Table 2](#) suggest that tidal effects on continuous monitoring data can severely violate assumptions required for methods of estimating ecosystem metabolism (as described in detail in Beck et al. 2015). These effects are easily identified by stronger correlations and lower RMSD using the detided dissolved oxygen. Further, effects of tidal advection can be seen with estimates from the Odum method as negative values for P and R, i.e., “anomalous” values. The effects of tidal advection on estimates from EBASE were more subtle as anomalous values cannot be returned based on constraints of the priors (i.e., none can be negative), although the range of values for the metabolic estimates were much larger with observed dissolved oxygen. A similar result (larger estimates for P and R) was observed using the synthetic time series with instrument and tidal noise ([Figure 7](#)). Overall, the results suggest that detiding the dissolved oxygen time series prior to estimating metabolic rates reduces tidal noise and produces more stable estimates with smaller ranges, regardless of the method used.

Discussion

The above analyses demonstrated that EBASE can successfully recover known metabolic parameters from a synthetic time series and provides robust estimates on real data covering a year of observations. The success of these results was predicated on the requirements of EBASE to address several critical needs that existing methods for estimating metabolism do not address for coastal applications. These needs were addressed primarily using a Bayesian framework that estimates the best fit of the model to the data with posterior probabilities describing the

likelihood of the fit. This framework enables hypothesis testing of how a model can be fit to data by using prior knowledge in the model fitting process, which results in posterior probabilities describing the certainty of the parameter estimates (Hilborn and Mangel 2013). The advantages of the Bayesian approach have led to widespread adoption over frequentist approaches in many scientific applications, especially in the coastal and marine community (e.g., Myers et al. 2001; Borsuk et al. 2001; Brown et al. 2017), yet these methods have not been rigorously explored for estimating metabolic rates in estuaries.

Our results demonstrated that even using uninformed priors, EBASE can reproduce known metabolic parameters and rates with reasonable certainty. However, initial analyses suggested an inability of the model to estimate stable values for the b parameter that influence gas exchange. This parameter was fixed for the sensitivity analyses and we were unable to evaluate the ability of EBASE to recover it from the synthetic time series. Future work should focus on understanding the sensitivity of EBASE to estimating b where the dominance of the relative processes that manifest signals in the dissolved oxygen time series could vary. For example, estuarine dissolved oxygen at Apalachicola Bay may be dominated by production and respiration, and less so from gas exchange, such that the available data may provide insufficient information for EBASE to estimate b . This aligns with others that have suggested gas exchange may be a relatively small component of the metabolic signal in shallow estuaries of the Gulf of Mexico (Murrell et al. 2018). In such cases, more constrained prior distributions for b could be appropriate or EBASE could be tested in settings with expected larger contributions of gas exchange expressed by dissolved oxygen. For application, users of EBASE may simply use a fixed value for b (e.g., $0.251 \text{ (cm hr}^{-1})/(\text{m}^2 \text{ s}^{-2})$) or perform a simple sensitivity analysis by varying b +/- a small percentage to determine how P and R may change. Further model

development may consider alternative approaches for dealing with equifinality, i.e., when the same modeled DO time series can be returned with different estimates of P , R , and D . Appling et al. (2018) provide a useful example for a stream metabolic model that addresses equifinality by allowing model parameters to vary with key drivers at sub-daily scales (e.g., gas exchange versus discharge) and avoiding assumptions that model residuals are uncorrelated.

Our results also confirmed that the effects of tidal advection on metabolic estimates can lead to biases in understanding gross primary production and ecosystem respiration. This result has previously been shown using the Odum open water method (Kemp and Boynton 1980; Caffrey 2003; Beck et al. 2015) and confirmed herein, whereby results using observed time series can produce over- and under-estimates of metabolic rates with more variation than those without tidal influence (Figures 7 and 8). As a result, detiding dissolved oxygen data is recommended prior to estimating metabolism, regardless of whether EBASE or an alternative method is used. In addition to inaccurate and imprecise metabolic estimates, tidal influences are also most likely observed as negative (or anomalous) values in the production and respiration rates using the Odum method (Caffrey 2003). Tidal effects may be less obvious using EBASE since negative values cannot be obtained based on constraints of the prior distributions, although as noted above, more variable estimates are returned. A potential future approach for developing EBASE could be an explicit formulation of tidal advection in the model using a synoptic tidal height time series in the Bayesian framework. Such an approach would have the advantage of simultaneously detiding and estimating metabolic rates using the same model, whereas using weighted regression prior to EBASE, as used herein, requires additional analysis and assumptions. However, field measurements (e.g., control volume approaches, Falter et al. 2008; Nidzieko et al.

2014) may be required to provide reasonable constraints on the prior distributions for any parameters that quantify advective influences on dissolved oxygen.

As described in the materials and procedures section, EBASE is an estuarine adaptation of BASE (Grace et al. 2015), which was developed for stream applications and some assumptions of the underlying model of the latter were inappropriate for the former. The most critical change made to BASE was adopting the gas transfer velocity parameterization in Wanninkhof (2014), which is primarily wind-based and more appropriate than the formulation in BASE. EBASE also removed the temperature dependency of respiration, consistent with applications of the Odum method to other shallow estuaries (Beck et al. 2015; Murrell et al. 2018). Overall, these changes also reduced the required inputs and many monitoring locations nationwide include the requisite data for applying EBASE (i.e., dissolved oxygen, water temperature, salinity, PAR, and wind speed, as collected by the NERRS). Further, EBASE could be applied to other non-tidal, lotic systems, although additional comparisons with existing methods are needed and the default uninformed prior distributions should be chosen carefully given the justification herein based primarily on estuarine literature (e.g., Caffrey 2004).

EBASE also provides several computational advantages over BASE implemented in the R package that was created for the purposes herein (Beck et al. 2024). Most importantly, EBASE was developed to allow different model optimization periods, whereas BASE was developed to estimate results for a single day. Allowing EBASE to incorporate more than a day of observations in the optimization can likely produce more accurate and precise estimates for the metabolic parameters. Physical and biological characteristics of an ecosystem that affect the metabolic rates are likely acting at time scales longer than a day, e.g., ecological and biogeochemical characteristics influencing the α and R parameters (such as community

composition and nutrient availability) may persist for several days. Exposing the model to additional observations may produce more stable results as the parameters for the best fit are estimated by the Bayesian routine as a function of the data that are evaluated each optimization period. However, we cannot provide a precise recommendation on the number of days to use for the optimization period as the exact length of time that ecosystem characteristics can affect metabolic rates may not be known and likely varies by location. Our example using the synthetic time series from Apalachicola Bay suggested that the most precise results were obtained using the 30 day optimization period, although results are likely to vary across systems. For most applications, very short (e.g., 1 day) or very long (e.g., > 30 days) are not recommended, such that the former may produce unstable results and the latter may miss important events in the time series producing parameters that are overly generalized. However, an advantage of the Bayesian approach is the ability to evaluate different optimization periods and, therefore, the amount of data on which to estimate key parameters. Hypotheses can be generated on the amount of time over which critical metabolic parameters may vary across systems. These hypotheses may relate to the length of time over which potential factors affect metabolism, e.g., storm events may affect metabolism at short time scales and a shorter optimization period could be used, whereas longer optimization periods may be more desirable if interested in long-term, climate-related effects on metabolism. These hypotheses may also consider frequency of continuous monitoring (e.g., 15 minute vs hourly) and how this may influence the results, as this is currently unknown for EBASE.

The EBASE R package can also accommodate missing observations in the input data. This feature allows the estimation of metabolic rates for time series that cover relatively long periods of time (e.g., more than year), when data gaps are likely to occur for several reasons (e.g.,

equipment malfunction and routine maintenance). The R package accommodates data gaps using linear interpolation for any required input used by EBASE, allowing the Bayesian routine to provide continuous estimates across the time series. The results are then automatically post-processed to remove any metabolic estimates that exceed a threshold for the number of interpolated observations. The analyst can determine the appropriate length of time to use for excluding results, although the default setting for EBASE is 12 hours, where results for an entire optimization period are removed if any interpolated period exceeded 12 hours within that period. Although this does not apply to the synthetic time series, some of the estimates using the 2021 observed data for Apalachicola Bay were excluded from the analysis. This feature allows EBASE to be applied more easily to other data sets because an analyst does not need to manually screen data that include missing values prior to analysis. More conservative gaps can be chosen if, for example, semidiurnal tidal signals operating at time scales less than 12 hours are expected to influence the results. However, detiding is strongly encouraged in these cases and the default gap size of 12 hours that describes the diurnal oxygen signal is likely appropriate after detiding.

While the EBASE theory and software provide advantages for metabolic estimates, the approach is not without limitations. Like most models, explicit choices are needed to apply EBASE to time series data. First, the use of unconstrained prior distributions was shown to reproduce known metabolic parameters with reasonable certainty, although initial assessments suggested the b parameter was relatively unstable and unconstrained priors may not provide useful estimates. Parameters that are poorly estimated may require constrained priors, although doing so may produce biased results in the absence of additional data to justify a constraint. Field-based measurements or alternative metabolic models could be used for informing priors. As an example, initial application of BASE to estuarine data prior to developing EBASE demonstrated

that unstable and unrealistic metabolic rates were returned with uninformed priors. The Odum method was used on the same data to develop an expectation of the range of values for the reaeration coefficient, K , which was then used to create an informed prior distribution for the same parameter using the BASE method. More stable and realistic metabolic estimates were then returned by BASE, demonstrating the value of the Bayesian approach that can incorporate prior knowledge. A similar approach using alternative metabolic models for informing priors could be applied to create more accurate estimates from EBASE. An additional choice for using EBASE is the model optimization period, although some guidance is provided above.

A final limitation of EBASE is the relatively long processing time when applying the method to a time series longer than a few days. For example, the execution time applying EBASE to a year of data on a conventional laptop computer was approximately 40 minutes, depending on the model settings. This time is compared to the Odum method applied to the same dataset, where results are obtained in a matter of seconds. Given the Bayesian framework used by EBASE, not considering the additional statistical advantages, it is not reasonable to expect comparable processing times between the methods. Regardless, computation times could be reduced with additional hardware improvements (e.g., accessing multiple processing cores) or changing the model estimation methods (e.g., reducing the number of MCMC simulations used by JAGS), although the latter may negatively affect model accuracy.

Comments and Recommendations

The development of EBASE represents a new approach for estimating metabolic rates in estuarine settings that leverages existing methods in a Bayesian framework. Our results have demonstrated that unknown metabolic parameters can be estimated with reasonable certainty and EBASE could be a valuable approach to improve the understanding of critical ecosystem

processes as the method can be readily applied to other settings. A notable limitation of EBASE was an inability to constrain the gas transfer velocity from a synthetic time series, although this result may be explained by a minimal contribution of gas exchange as expressed in the dissolved oxygen time series. Effects of tidal advection on dissolved oxygen measurements were also observed, demonstrating a violation of the assumption that the measured data represent a water sample having a continuous metabolic history. Further development of EBASE to accommodate a tidal signal, or exploring alternative methods for detiding dissolved oxygen data, are promising avenues of future research to more accurately quantify metabolic parameters in estuaries. Overall, EBASE represents a potentially powerful tool that removes many of the assumptions of existing methods by allowing unknown metabolic parameters to be estimated by the data and can also incorporate existing knowledge for further exploration of estuarine ecosystem properties.

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793

Figure Legends

Figure 1: The default prior distributions for α , R , and b used in EBASE. All priors are normal distributions and truncated to positive values. b is also truncated to a maximum of 0.502 ($\text{cm hr}^{-1})/(\text{m}^2 \text{ s}^{-2})$. Probabilities have been normalized to the maximum probability.

Figure 2: Synthetic time series for one year of continuous data at Apalachicola Bay. Synthetic data were created using the (a) a parameter to estimate (b) metabolic estimates for gross primary production (P), ecosystem respiration (R), and gas exchange (D) and the (c) dissolved oxygen time series (including saturation, C_{sat}).

Figure 3: Comparison of EBASE results using default prior distributions to a synthetic time series created with known model parameters (α , R , and b). Results are compared for EBASE parameters estimated with a (a) 7 day and (b) 30 day optimization period. 95% credible intervals from the posterior distributions of the parameter estimates from EBASE are also shown.

Figure 4: Comparison of EBASE results to a synthetic time series created with known model parameters (α , R , and b). Results are compared for unique combinations of prior distributions and optimization period. The means (μ) and standard deviations (σ) are evaluated as low (L) or high (H) values (see text for details) and the optimization period for EBASE is 1 day, 7 days, or 30 days. The model predictions of dissolved oxygen (DO), gross primary production (P), ecosystem respiration (R), air–water oxygen flux (D), and light efficiency (α) are evaluated based on Nash–Sutcliffe Efficiency (NSE) values between the EBASE results and synthetic values. The b parameter is a fixed constant and was not evaluated. Rankings of each combination as the median NSE value across all five model outputs in a row are shown on the right, with the top three as black/bold and bottom three as black/italic.

Figure 5: Comparison of EBASE results for the best and worst performing models to a synthetic time series created with known metabolic parameters. The best and worst performing models for the 1 day (a, b), 7 day (c, d), and 30 day (e, f) optimization periods are based on the EBASE results with prior distributions that produced the highest and lowest median Nash–Sutcliffe Efficiency values across all parameter estimates (Figure 4). The results are averaged at the time step of the model optimization period.

Figure 6: A subset of the synthetic time series (Figure 2c) and the synthetic time series with noise for evaluating the ability of EBASE to recover known metabolic parameters. The (a)

estimated residual and tidal noise added to the (b) synthetic time series are shown.

800

Figure 7: Comparisons of EBASE to recover parameters α (top) and R (bottom) from a synthetic time series and a synthetic time series with residual and tidal noise included. The left plots show the time series and the right plots show a 1:1 comparison for each result. See [Figure 6](#) for subsets of both dissolved oxygen time series.

801

Figure 8: Comparisons of daily metabolic estimates from the EBASE and Odum methods for one year of continuous monitoring data at Apalachicola Bay. Results for (a) gross primary production (P), (b) ecosystem respiration (R), and (c) net ecosystem metabolism (NEM) are compared using the observed and detided dissolved oxygen time series as input to each model. Black lines show the 1:1 comparison and the red lines show the linear regression fit.

802

803 **Tables**

Table 1: EBASE model parameters showing the required input, parameters derived from the model input, and model output.

Type	Description	Model notation	Units
Input	Dissolved oxygen (observed)	C	mmol m^{-3}
	Water temperature	-	$^{\circ}\text{C}$
	Salinity	-	psu
	Total photosynthetically active radiation	PAR	W m^{-2}
	Wind speed	-	m s^{-1}
	Water column depth (mean or tidal height vector)	Z	m
Input-derived	Wind speed at 10 meter height, squared	U_{10}^2	$\text{m}^2 \text{s}^{-2}$
	Schmidt number (from water temperature and salinity)	Sc	unitless
	Dissolved oxygen at saturation (from water temperature and salinity)	C_{sat}	mmol m^{-3}
Output	Dissolved oxygen (modelled)	C_{mod}	mmol m^{-3}
	Production	P	$\text{mmol m}^2 \text{d}^{-1}$
	Respiration	R	$\text{mmol m}^2 \text{d}^{-1}$
	Gas exchange	D	$\text{mmol m}^2 \text{d}^{-1}$
	Light efficiency	a	$(\text{mmol m}^2 \text{d}^{-1})/(\text{W m}^{-2})$
	Sensitivity of gas transfer to wind speed	b	$(\text{cm hr}^{-1})/(\text{m}^2 \text{s}^{-2})$

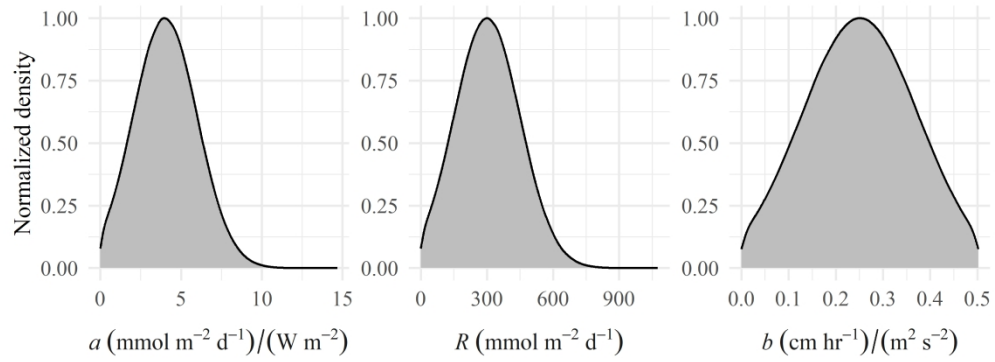
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Table 2: Summary statistics of daily metabolic estimates comparing the EBASE and Odum methods for gross primary production (P), ecosystem respiration (R), and net ecosystem metabolism (NEM) using the observed (left values) and detided (right values) dissolved oxygen time series as input to each model. Summary statistics include Pearson correlation coefficients and root mean square difference (RMSD) between the metabolic estimates obtained from each method. P-values for correlation coefficients all less than 0.005.

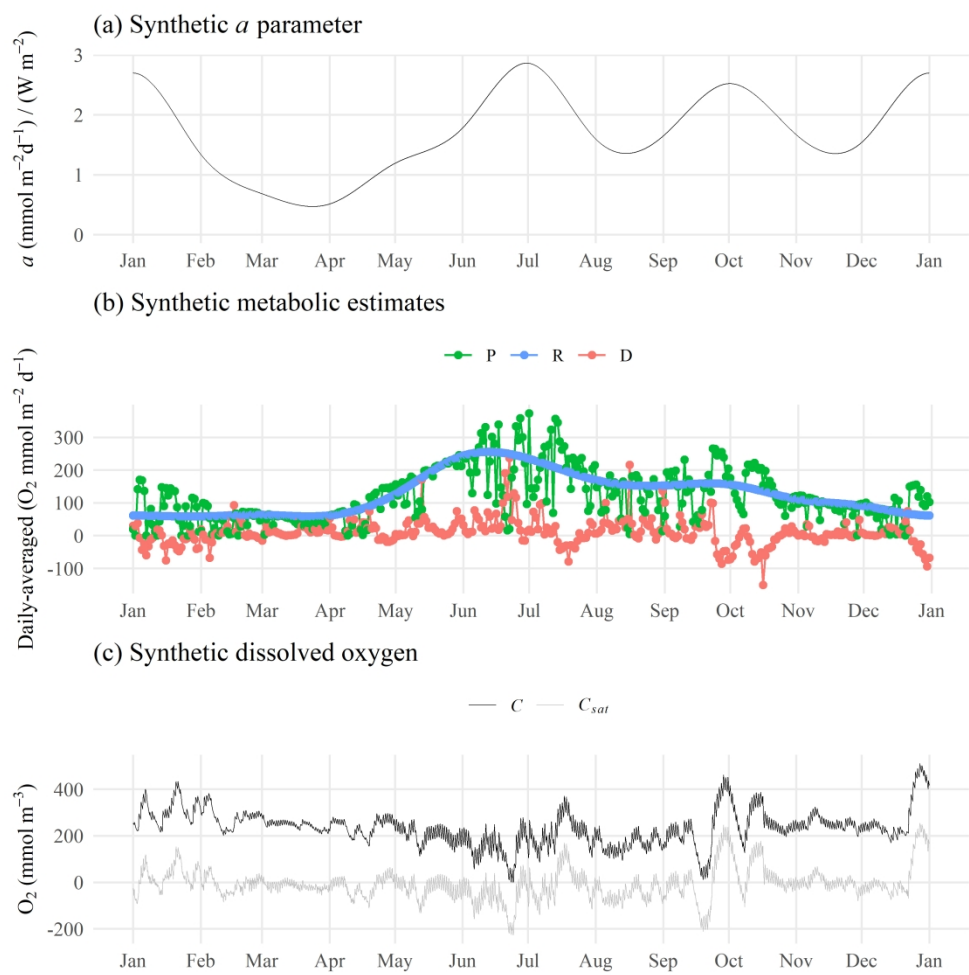
Parameter	ρ	RMSD (mmol O ² /m ² /d)
P	0.7 / 0.71	76.17 / 14.9
R	0.51 / 0.49	98.76 / 27.29
NEM	0.36 / 0.52	42.28 / 17.98

805

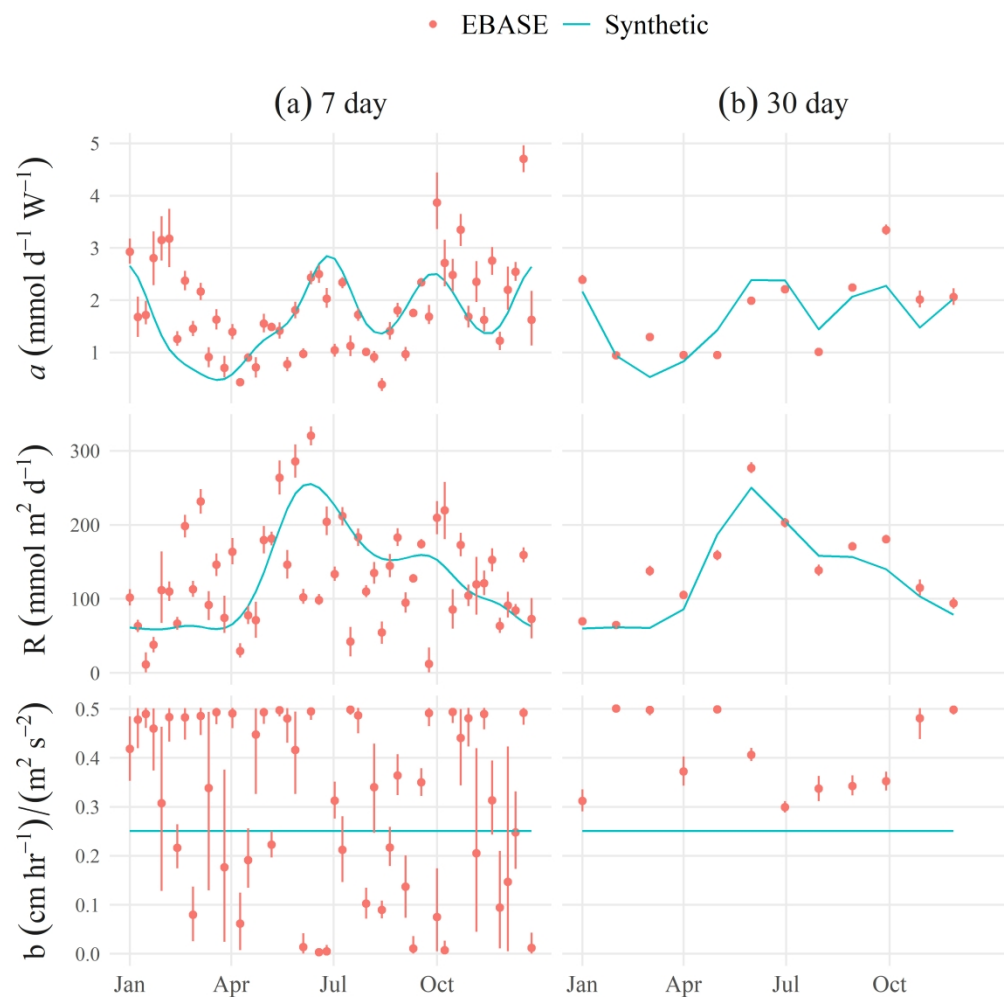
For Review Only



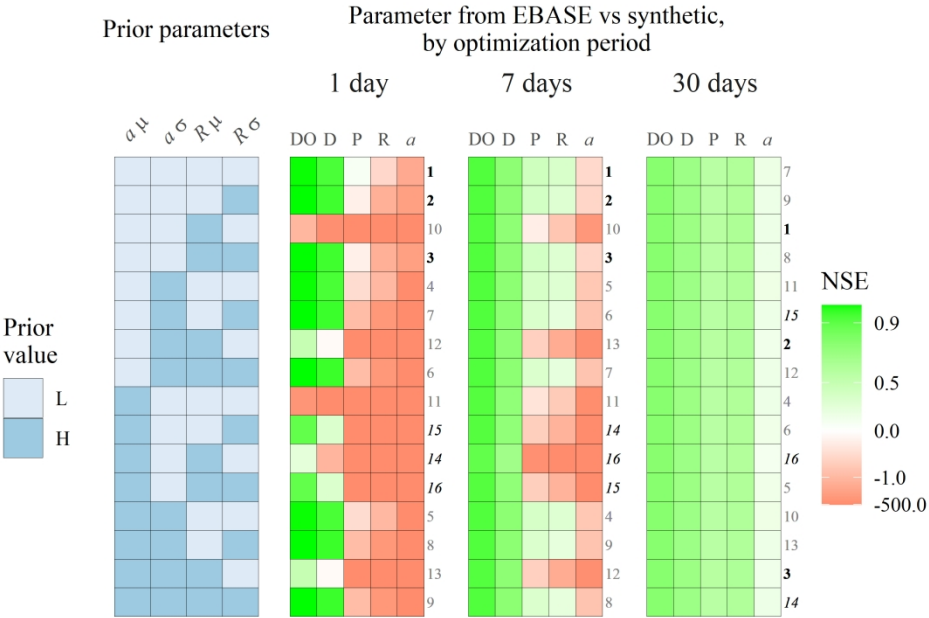
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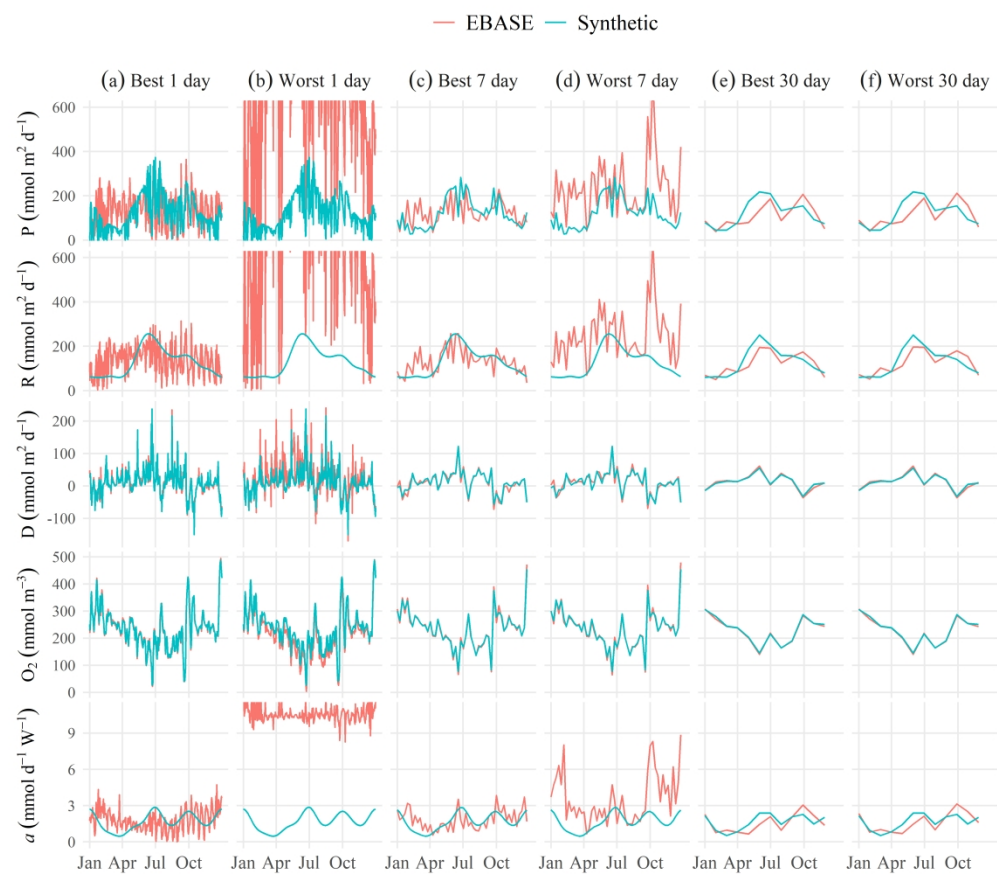
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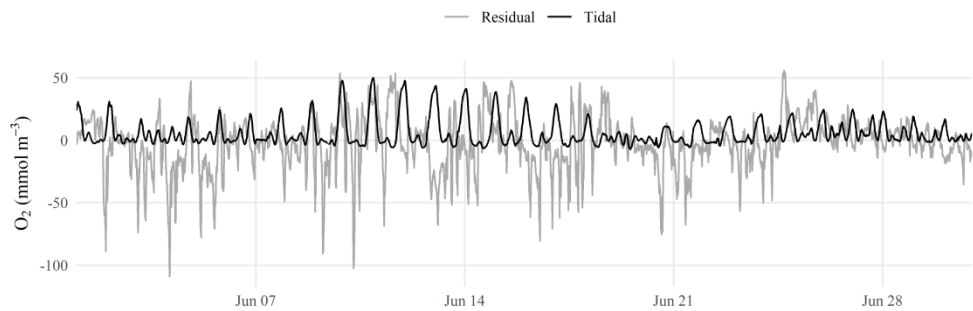


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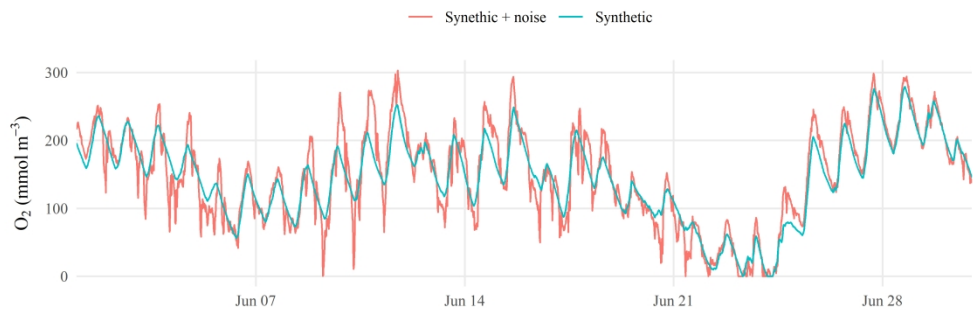


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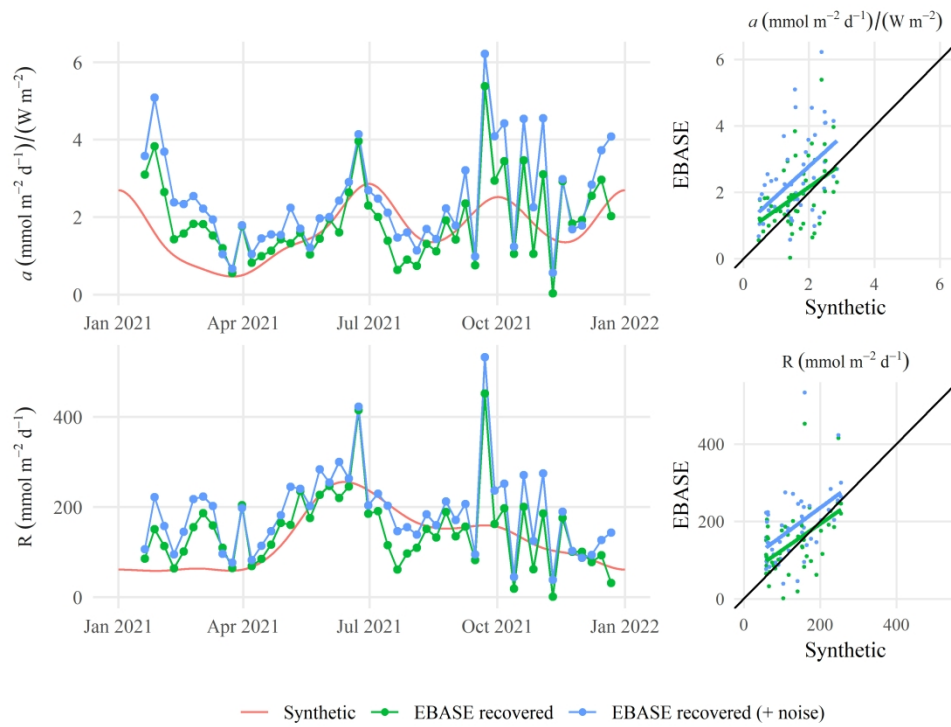
(1) Noise



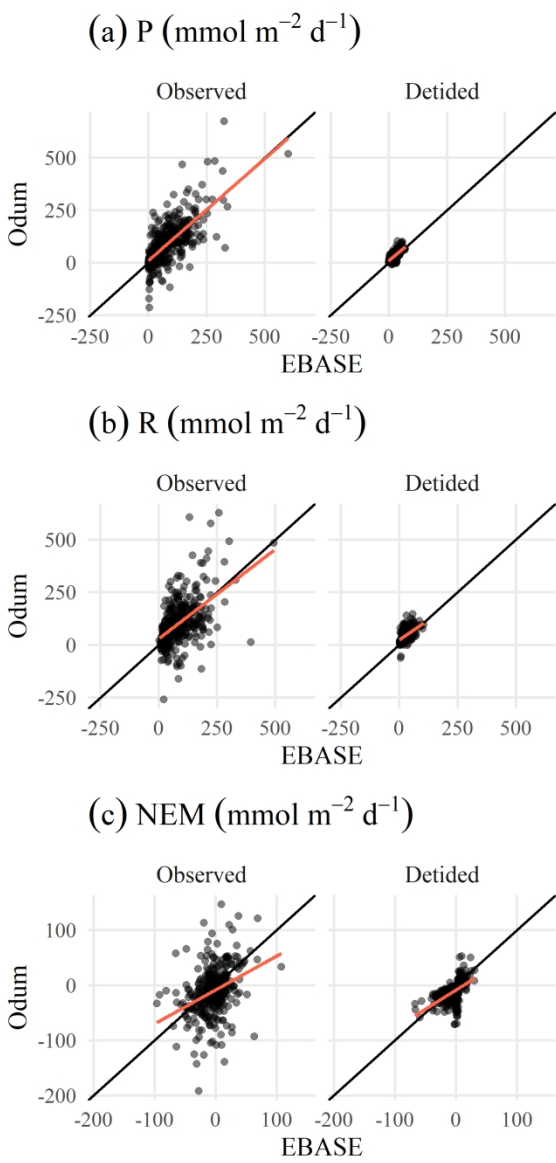
(b) Time series



515x386mm (197 x 197 DPI)



451x354mm (197 x 197 DPI)



225x451mm (197 x 197 DPI)