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Methods of approximation influence aquatic ecosystem metabolism estimates

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Abstract

Aquatic ecologists have recently employed dynamic models to estimate aquatic ecosystem metabolism. All approaches involve numerically solving a differential equation describing dissolved oxygen (DO) dynamics. Although the DO differential equation can be solved accurately with linear multistep or Runge–Kutta methods, less accurate methods, such as the Euler method, have been applied. The methods also differ in how discrete temperature and light measurements are used to drive DO dynamics. Here, we used a representative stream DO data set to compare the metabolism estimates generated by multiple Euler based methods and an accurate numerical method. We also compared metabolism estimates using linear, piecewise constant and smoothing spline interpolation of light and temperature. Using observed DO to calculate DO saturation deficit in the Euler method results in a substantial difference in metabolism estimates compared to all other methods. If modeled DO is used to calculate DO saturation deficit, the Euler method introduces smaller error in metabolism estimates, which diminishes as logging interval decreases. Linear and smoothing spline interpolation result in similar metabolism estimates, but differ from estimates based on piecewise constant interpolation. We demonstrate how different computational methods imply distinct assumptions about process and observation error, and conclude that under the assumption of observation error, the best practice is to use the accurate numerical method of solving differential equation with a continuous interpolation of light and temperature. The Euler method will introduce minimal error if it is paired with frequently logged data and DO saturation deficit is computed using modeled DO.

For well over a half century, aquatic gross primary production (GPP) and ecosystem respiration (ER) have been estimated from open–water dissolved oxygen (DO) measurements. H. T. Odum first proposed using diel changes in DO concentration to parse the autotrophic and heterotrophic components of whole ecosystem metabolism (Odum 1956). He realized that after accounting for air–water exchange, often referred to as reaeration, DO changes at night are solely due to ER and DO changes during the day reflect the difference between DO production from GPP and DO consumption via ER. However, accurately accounting for reaeration, which is critical for obtaining accurate estimates of GPP and ER, is far from trivial. Since Odum's seminal contribution, the open channel method has been refined and improved, primarily in efforts to accurately account for reaeration. One approach to account for reaeration is to estimate the reaeration coefficient using a certain portion of the diel DO curve. For example, Hornberger and Kelly (1975) proposed regressing night time changes in DO on DO saturation deficit as a way to calculate the reaeration coefficient (the slope of this regression) simultaneously with ER (the intercept of this regression). Chapra and Di Toro (1991) showed that the reaeration coefficient is functionally linked to the time lag between solar noon and maximum DO deficit and proposed the so called delta method to estimate the reaeration coefficient from this functional relationship. Another approach is predicting reaeration coefficients from physical characteristics of the environment such as stream channel morphology and velocity (Tsivoglou and Neal 1976; Melching and Flores 1999; Raymond et al. 2012), or wind speed (Wanninkhof 1992; Clark et al. 1995; Cole and Caraco 1998; Crusius and Wanninkhof 2003; Jonsson et al. 2008). A third approach is to experimentally determine reaeration coefficients using gas tracer injections (Wanninkhof 1992;

Additional Supporting Information may be found in the online version of this article.

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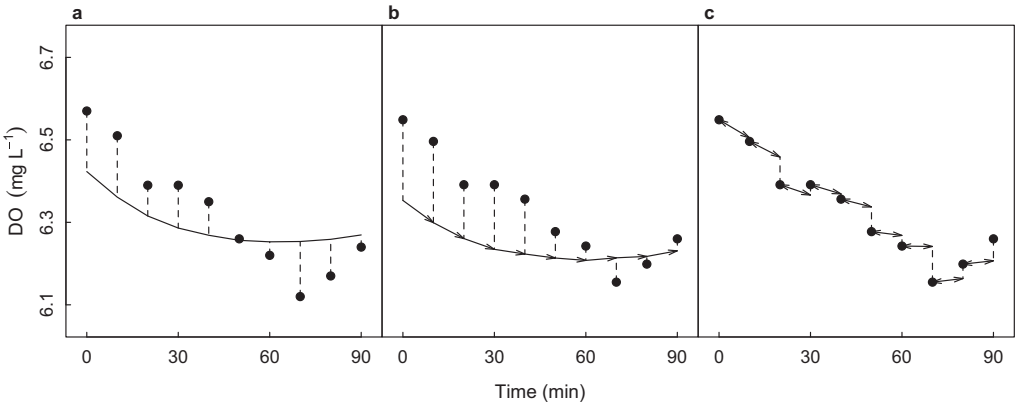

Fig. 1. Schematics of different methods of solving the differential equation for dissolved oxygen dynamics. (a–c) are illustrations of the accurate method, Euler method and the stepwise method, respectively. Vertical dashed lines indicate the difference between measured and modeled DO concentration (a, b) or DO concentration changes between successive measurements (c). Points in the graphs are measured DO concentration. Lines and arrows represent the modeled DO concentration (a, b) or DO concentration changes between successive measurements (c). DO data plotted in this figure are a subset of the data used in this article.

Marzolf et al. 1994; Cole and Caraco 1998; Young and Huryn 1998) or floating chambers (Marino and Howarth 1993; Kremer et al. 2003; Borges et al. 2004).

However, all approaches have shortcomings. Estimating reaeration coefficients based on characteristics of a certain portion of the diel DO curve does not account for the temperature dependence of GPP, ER and reaeration. Predicting reaeration coefficients based on physical characteristics of the environment is often site and time specific, and cannot be applied generally. Experimentally measuring reaeration coefficients is time consuming and single measurement does not represent the reaeration coefficient over time due to its dependency on the flow conditions. The location where reaeration coefficients are measured also may not necessarily correspond to the area driving measured DO concentration. In addition, the relationship between reaeration coefficients of different gases is not theoretically well defined in the presence of bubbles. Failure to accurately estimate reaeration can easily lead to biased GPP and ER estimates.

To tackle the problem of accurately accounting for reaeration, several researchers recently proposed the application of dynamic models to estimate aquatic ecosystem metabolism (Van de Bogert et al. 2007; Hanson et al. 2008; Holtgrieve et al. 2010; Riley and Dodds 2013; Solomon et al. 2013; Grace et al. 2015). Although it has its own challenges, such as difficulty in separating GPP, ER and reaeration in high turbulent systems (Demars et al. 2015), the dynamic modeling approach has several advantages compared to the traditional methods based on oxygen budgets (Holtgrieve et al. 2015). It allows simultaneous quantification of reaeration, GPP and ER, and enables the mechanistic characterization of GPP, ER and reaeration that explicitly captures the environmental dependency of these processes. Additionally, with assumptions about error distribution, confidence can be ascribed to model parameters and GPP and ER estimates. Furthermore, if a Bayesian approach is taken, prior knowledge about parameters related to GPP, ER and reaeration can be formally incorporated.

Fitting a dynamic model to observed DO data usually involves the following steps:

1. Formalize the differential equation describing DO changes over time.

$$\frac{d[O_2]}{dt} = P(I,T) - R(T) + K(T)\left([O_2]_{sat} - [O_2]\right) \quad (1)$$

   Here, $[O_2]$ is DO concentration. $[O_2]_{sat}$ is the DO concentration at saturation, which can be calculated based on barometric pressure and temperature. $P(I,T)$, $R(T)$ and $K(T)$ are GPP, ER and reaeration coefficient, respectively. Often, we describe GPP as a function of light (I) and temperature (T), ER as a function of T, and reaeration coefficient as a function of T. Parameters in the functions $P(I,T)$, $R(T)$ and $K(T)$ are the parameters to be estimated in the model.
2. For a given set of parameters, solve Eq. 1 to obtain the modeled DO concentration (Fig. 1a).
3. Calculate the differences between modeled and measured DO concentration. The differences between modeled and measured DO concentration are often assumed to be independent and identically distributed normal random variables. With such a distributional assumption, the likelihood for a given set of parameters in the differential equation can be computed.
4. Either find the maximum likelihood estimates of parameters by iterating step 2–3 to find the parameters that maximize the likelihood, or employ a computational Bayesian approach to obtain the posterior distributions of the parameters.

Solving Eq. 1 analytically is usually infeasible with the typical GPP, ER and reaeration formulations unless specific functional forms are used to approximate daily light and temperature (Reichert et al. 2009). Thus, numerical methods are usually necessary. Conceptually, numerical methods approximate the solution by discretizing continuous time into steps. A numerical method starts from an initial point and moves a short step forward in time to find the solution at the next time point. Numerical integration using Runge–Kutta methods or linear multistep methods can accurately simulate Eq. 1. The accuracy comes from using derivatives at several intermediate steps (Runge–Kutta methods) or the linear combination of derivatives at several previous time steps (linear multistep method) to find the solution at the next time point. For example, for a differential equation $dy(t)/dt=f(t)$, a second order Adams method approximates the solution as $y(t+\Delta t)=y(t)+\left(\frac{3}{2}f(t)-\frac{1}{2}f(t-\Delta t)\right)\Delta t$. A second order backwards differentiation formula approximates the solution as $y(t+\Delta t)=\frac{4}{3}y(t)-\frac{1}{3}y(t-\Delta t)+\frac{2}{3}\Delta t f(t+\Delta t)$. The accuracy of these methods can be enhanced by incorporating more steps in the solution. Due to their greater accuracy over Euler based methods, which approximate the solution as $y(t+\Delta t)=y(t)+\Delta t f(t)$, we refer to these methods collectively as the accurate method. Although the accurate numerical integration method (Runge–Kutta method in this case) has been applied in a stream metabolism study (Holtgrieve et al. 2010), aquatic ecologists have commonly employed simpler, computationally faster, but less accurate numerical methods such as the Euler method (Hall and Tank 2005; Van de Bogert et al. 2007; Hanson et al. 2008; Bernot et al. 2010; Solomon et al. 2013; Hotchkiss and Hall 2014) to solve Eq. 1. The Euler method is a first order approximation, discretizing the differential equation with a fixed time step to obtain a solution (Fig. 1b). It is computationally fast and easy to implement. The approximated trajectory of DO concentration using this approach is given by

$$[O_2]_{\text{modeled},t+\Delta t}=[O_2]_{\text{modeled},t}+\Delta t\left(P(I_t,T_t)-R(T_t)+K(T_t)\left([O_2]_{\text{sat},t}-[O_2]_{\text{modeled},t}\right)\right) \quad (2)$$

Here, the subscript t denotes time, and Δt is the fixed time step often corresponding to the logging interval for DO concentration. Recently, Hall et al. (2015) modified Euler method to include the average of modeled DO concentration at the beginning and end of the logging interval in the calculation of DO saturation deficit. Applying their method, the approximated trajectory of DO concentration is given by

$$[O_2]_{\text{modeled},t+\Delta t}=[O_2]_{\text{modeled},t}+\Delta t\left(P(I_t,T_t)-R(T_t)+K(T_t)\left([O_2]_{\text{sat},t}-\frac{[O_2]_{\text{modeled},t}+[O_2]_{\text{modeled},t+\Delta t}}{2}\right)\right) \quad (3)$$

which can be rearranged to facilitate recursive prediction of DO concentration as:

$$[O_2]_{\text{modeled},t+\Delta t}=\frac{[O_2]_{\text{modeled},t}+\Delta t(P(I_t,T_t)-R(T_t)+K(T_t)([O_2]_{\text{sat},t}-\frac{1}{2}[O_2]_{\text{modeled},t}))}{1+\frac{1}{2}K(T_t)\Delta t} \quad (4)$$

Another approach in the aquatic metabolism literature utilizes the Euler method, but differs in that measured DO instead of modeled DO is used to calculate DO saturation deficit (Grace et al. 2015). The approximated trajectory of DO concentration is given by

$$[O_2]_{\text{modeled},t+\Delta t}=[O_2]_{\text{modeled},t}+\Delta t\left(P(I_t,T_t)-R(T_t)+K(T_t)\left([O_2]_{\text{sat},t}-[O_2]_{\text{measured},t}\right)\right) \quad (5)$$

which can be rearranged as

$$\Delta[O_2]_{\text{modeled},t}=[O_2]_{\text{modeled},t+\Delta t}-[O_2]_{\text{modeled},t}+\Delta t\left(P(I_t,T_t)-R(T_t)+K(T_t)\left([O_2]_{\text{sat},t}-[O_2]_{\text{measured},t}\right)\right) \quad (6)$$

Equation 6 was implemented in a recent methods paper (denoted here as the stepwise method) and was phrased as modeling the changes in DO concentration between successive measurements (Grace et al. 2015) (Fig. 1c). Although Eqs. 5 and 6 represent the same method in different forms, modeling DO concentration ($[O_2]$) or changes in DO concentration between measurements ($\Delta[O_2]=[O_2]_{t+\Delta t}-[O_2]_t$) often involves different assumptions about error distribution, and can influence inference about stream metabolism. If we assume that the difference between measured and modeled changes in DO concentration between successive measurements are independent and identically distributed normal variables ($\Delta[O_2]_{\text{measured},t}-\Delta[O_2]_{\text{modeled},t}\sim N(0,\sigma^2)$), the differences between measured and modeled DO concentration ($[O_2]_{\text{measured},t}-[O_2]_{\text{modeled},t}$) will be correlated. Thus assuming independent and identically distributed normal observation error between modeled and measured DO concentration (using Eq. 5, assuming $[O_2]_{\text{measured},t}-[O_2]_{\text{modeled},t}\sim N(0,\sigma^2)$) can result in different estimates than those obtained from assuming independent and identically distributed normal observation error between modeled and measured changes in DO concentration between successive measurements (using Eq. 6, assuming $\Delta[O_2]_{\text{measured},t}-\Delta[O_2]_{\text{modeled},t}\sim N(0,\sigma^2)$).

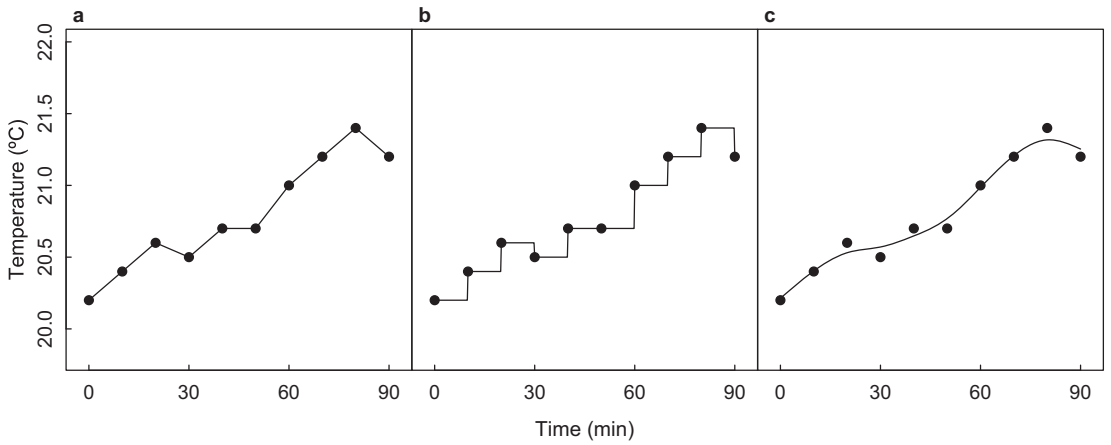

Fig. 2. Schematics of different methods of interpolating light and temperature data. (a–c) are illustrations of linear interpolation, piecewise constant interpolation and smoothing spline interpolation, respectively. Temperature data plotted in this figure are a subset of the data used in this article.

The three methods, accurate, Euler and stepwise methods, for solving differential equation differ in four important ways. The first key difference is the accuracy achieved with each method. The accurate method yields a very accurate solution because it uses information from several time steps. The Euler and stepwise methods use a fixed step size, and only employ first order derivative at one step to approximate solutions. Such an approximation will introduce error and thus the solution to a differential equation obtained using Euler based methods will typically be different from solutions obtained using accurate approaches. The second difference among the three methods is whether modeled or measured DO concentration is used in the calculation of reaeration. The accurate and Euler methods use modeled DO concentration to calculate reaeration, whereas the stepwise method uses measured DO concentration. The third important difference among the three methods is how light and temperature are interpolated between discrete observations. In the Euler and stepwise methods, only light and temperature at the time of each DO measurement are used to drive changes in DO, and thus a piecewise constant interpolation of light and temperature between measurement times (Fig. 2b) is implicitly assumed. When using the accurate method, exogenous drivers must be continuous, and therefore light and temperature must be interpolated between measurements. Common methods of interpolation include linear interpolation (Fig. 2a), piecewise constant interpolation (Fig. 2b), and smoothing spline interpolation (Fig. 2c). The fourth important difference is the assumption about the distribution of error. Usually, the stepwise method assumes that the differences between modeled and measured changes in DO concentration between successive measurements are independent and identically distributed normal random variables ($\Delta[O_2]_{\text{measured},t} - \Delta[O_2]_{\text{modeled},t} \sim N(0, \sigma^2)$), which implies that the differences between measured and modeled DO concentration are correlated normal random variables. This is different than the assumption of independent and identically distributed random difference between modeled and measured DO concentration ($[O_2]_{\text{measured},t} - [O_2]_{\text{modeled},t} \sim N(0, \sigma^2)$).

Although it is well known that methods of approximating solutions to differential equations introduce error, how such error influences metabolism estimates has not been evaluated. In this study, we use a representative stream DO dataset to evaluate the error associated with Euler and stepwise methods by comparing the resulting metabolism estimates to those obtained from the accurate method. For the accurate method, we also evaluate how methods of interpolating light and temperature influence metabolism estimates.

Assessment

Data

We collected data to estimate whole stream metabolism in lower Kings Creek (39.10004˚N, 96.60959˚W) located within the Konza Prairie Biological Station near Manhattan, Kansas, U.S.A. Specifically, we recorded DO concentration, water temperature and barometric pressure using a YSI ProODO handheld optical DO meter (YSI Instruments, Yellow Springs, Ohio, U.S.A.) and photosynthetically active radiation (PAR) using an Odyssey Irradiance logger (DataFlowSystems, Christchurch, New Zealand) at a single location in the stream every 10 min for 8 consecutive days (28 May–05 June 2013). The DO meter was calibrated with water saturated air prior to deployment and the irradiance logger was converted to PAR using a conversion coefficient derived from comparison to a calibrated PAR sensor.

Metabolism calculation

We simultaneously quantified reaeration, GPP and ER from the diel changes in DO concentration measured at a single location in the stream. Changes in DO concentration can be generally described by Eq. 1, which we specified using the formulae adopted by Riley and Dodds (2013).

Specifically, we calculated the $[O_2]_{sat}$ as follows (American Public Health Association 1995).

$$[O_2]_{\text{sat}} = e^{-139.3441+\frac{157570}{T+273.15}-\frac{66423080}{(T+273.15)^2}+\frac{12438000000}{(T+273.15)^3}-\frac{862194900000}{(T+273.15)^4}} \times \frac{\text{Pa}\times 0.998}{101.3} \quad (7)$$

where T is temperature (°C) and Pa is barometric pressure (kPa). The reaeration coefficient K is temperature corrected (Elmore and West 1961; Bott 2006) based on the following formula:

$$K(T) = K_{20} \times 1.024^{T-20} \quad (8)$$

where K_{20} is the reaeration coefficient at 20°C. We modeled respiration rate as a temperature dependent process (Gulliver and Stefan 1984; Parkhill and Gulliver 1999)

$$R(T) = R_{20} \times 1.045^{T-20} \quad (9)$$

where R_{20} is the respiration rate at 20°C. We modeled photosynthesis rate as a saturating function of light (Jassby and Platt 1976) with temperature dependence (Megard et al. 1984)

$$P(I,T) = P_{\max} \tanh\left(\frac{\alpha I}{P_{\max}}\right) \times 1.036^{T-20} \quad (10)$$

I is PAR (μE m^{-2} s^{-1}), α is the slope of the photosynthesis–light relationship at low light intensity, and $P_{\max}$ is the photosynthesis rate at light saturation. In this formulation of Eq. 1, I and T are from field measurements and $P_{\max}$, α, R_{20} and K_{20} are parameters to be estimated. Although researchers have chosen different formulations of the model, the shape of $R(T)$ and $P(I,T)$ are generally similar. Therefore, our particular choice of model formulation should result in no loss of generality when comparing the influences of computation methods on metabolism estimates.

We used the three methods described above, Euler, stepwise and accurate, to simulate Eq. 1 and provided modeled DO (Euler and accurate methods) or changes in DO (stepwise method) for a particular set of parameters. Interpolating light and temperature was unnecessary for the Euler and stepwise methods because both methods only use light and temperature data at the time of each DO measurement. Therefore, we only compared the three methods of interpolation, linear (Fig. 2a), piecewise constant (Fig. 2b), and smoothing spline (Fig. 2c), using the accurate numerical method. In total, we compared parameter estimates and daily GPP and ER estimates using five methods with the same data set: stepwise method, Euler method and accurate method with three different ways of interpolating light and temperature.

We implemented the accurate method using the differential equation solver lsoda in the R package deSolve (Soetaert et al. 2010). The function lsoda implements linear multistep methods to solve differential equations with high accuracy. Specifically, the function automatically selects between the Adams method and the backwards differentiation formula method by dynamically monitoring the data (Hindmarsh 1983; Petzold 1983). The three methods of interpolation were implemented as illustrated in Fig. 2a–c. For the linear interpolation, we assumed that light/temperature changed linearly between logging intervals (Fig. 2a). For piecewise constant interpolation, we assumed constant light/temperature between logging intervals equal to the measurement made at the beginning of each logging interval (Fig. 2b). For the smoothing spline interpolation, we first fit a cubic smoothing spline between light/temperature and time, and then used the fitted smoothing spline to represent light/temperature over time (Fig. 2c). We implemented the linear interpolation and piecewise constant interpolation using function approxfun and smoothing spline interpolation using function smooth.spline in R. We used the default number of knots in function smooth.spline. For the 10 min logging interval, we used 153 knots for 1153 light/temperature measurements, and for the 30 min logging interval, we used 116 knots for 384 light/temperature measurements. For the Euler method, we used Eq. 2 and the logging interval of DO data as the step size Δt. We also evaluated whether slight modifications to Euler method could improve its accuracy. We implemented the modified Euler method by Hall et al. (2015) and applied this method to the same data set with 10 min logging interval following Eq. 4. For the stepwise method, we used Eq. 6 to model the changes in DO concentration between successive measurements because this is the commonly implemented form when measured DO is used to compute DO saturation deficit (sensu Grace et al. 2015). We used measured DO concentration to calculate reaeration in the stepwise method, whereas we used modeled DO in the Euler and accurate methods. Finally, we explored how the differences in metabolism estimates among methods change with the logging interval of DO data because error associated with approximate methods increases with step size of time. To this end, we subsampled the data every 30 min and performed the same estimation with the five methods discussed above.

We employed a Bayesian approach to estimate parameters and daily GPP and ER with each of the methods. For a given set of parameters, we numerically solved Eq. 1 with the five methods discussed above, and obtained a trajectory of modeled DO concentration (accurate method and Euler method) or modeled changes in DO concentration between successive measurements (stepwise method). We assumed that the differences between modeled and measured DO (accurate method and Euler method) or changes in DO concentration between successive measurements (stepwise method) were independent and identically distributed normal random variables. It is worth noting that such an assumption about independence of error might be a simplification of reality,

Table 1. Assumptions used in various methods. Columns correspond to different assumptions about error distribution. $[O_2]_{\text{measured},t} - [O_2]_{\text{modeled},t} \sim N(0, \sigma^2)$ refers to the assumption that difference between measured and modeled DO concentration are independent and identically distributed random variables. $\Delta[O_2]_{\text{measured},t} - \Delta[O_2]_{\text{modeled},t} \sim N(0, \sigma^2)$ refers to the assumption that differences between measured and modeled changes in DO concentration between successive measurements are independent and identically distributed random variables. Rows correspond to whether measured or modeled DO concentration is used to calculated DO saturation deficit.

	$[O_2]_{\text{measured},t} - [O_2]_{\text{modeled},t} \sim N(0, \sigma^2)$	$\Delta[O_2]_{\text{measured},t} - \Delta[O_2]_{\text{modeled},t} \sim N(0, \sigma^2)$
Measured DO	Stepwise variant 2	Stepwise
Modeled DO	Accurate, Euler	Stepwise variant 1

and consequently, we may underestimate the uncertainty associated with parameters and metabolism. The distributional assumption of error provided the basis to compute the likelihood for any given set of parameters. We used uniform priors for all the parameters in the model. We set the lower bound of the uniform prior at 0 and the upper bound at values significantly larger than found in the literature for all parameters. We used Markov Chain Monte Carlo (MCMC) to sample the posterior distribution of the parameters. Specifically, we employed the adaptive random walk Metropolis–Hasting algorithm (Haario et al. 2001) with the function metrop in the R package mcmc (Geyer and Johnson 2014). We performed visual inspection and Geweke diagnostics (Geweke 1992) of the trace plots to ensure the convergence of the Markov Chains.

To obtain posterior distributions of GPP and ER, we calculated the corresponding metabolism rates from each combination of parameters in each Markov chain. More specifically, we numerically integrated the instantaneous rates of GPP and ER over time. With the Euler and stepwise methods, the numerical integration simplified to a summation; instantaneous rates at each measurement time were multiplied by the logging interval to compute the GPP and ER for all intervals. We then obtained the daily GPP and ER by summing over all the intervals in a day. We performed the same diagnostics of Markov chains to ensure convergence. We reported the average daily GPP and ER over the 8 d.

For both parameter estimates and daily GPP and ER estimates, we computed posterior means and 95% highest posterior density intervals using the R package coda (Plummer et al. 2006). To compare parameter or daily GPP and ER estimates from different methods, we examined whether the 95% highest posterior density intervals overlapped or not. All computation and data analyses were performed in R 3.2.0 (R Core Team 2015). The R code for all methods are supplied as Supporting Information.

We implemented two variants of the stepwise method to evaluate how using measured DO concentration and how making different distributional assumptions about error each influence parameter and daily GPP and ER estimates (Table 1). In the first variant (referred to as stepwise variant 1), we used modeled DO to calculate DO saturation deficit, but assumed independent and identically distributed normal error between modeled and measured changes in DO concentration between successive measurements ($\Delta[O_2]_{\text{measured},t} - \Delta[O_2]_{\text{modeled},t} \sim N(0, \sigma^2)$). An alternative way of describing this variant of the stepwise method is that we modeled DO concentration using the Euler method as prescribed in Eq. 2, but instead of comparing measured and modeled DO concentration, we compared the measured and modeled changes in DO concentration between successive measurements, assuming that differences were independent and identically distributed normal random variables. In the second variant (referred to as stepwise variant 2), we used measured DO concentration to calculate DO saturation deficit and obtained the trajectory of modeled DO concentration according to Eq. 5. We assumed that the difference between modeled and measured DO concentrations were independent and identically distributed normal variables ($[O_2]_{\text{measured},t} - [O_2]_{\text{modeled},t} \sim N(0, \sigma^2)$). We applied these two variants of stepwise method to the data with a 10 min logging interval, and employed the same computational Bayesian approach to obtain parameter and daily GPP and ER estimates.

Results

The different computational methods for modeling aquatic metabolism yielded substantially different parameter estimates as well as daily GPP and ER estimates. Parameter estimates (Fig. 3) and estimated daily GPP and ER (Fig. 4) using the stepwise method were dramatically different from all other methods, irrespective of logging interval. Both variants of the stepwise method underestimated parameters and daily GPP and ER compared to the Euler and accurate methods (Supporting Information Table A4). While the stepwise method and both variants fit the changes in DO concentration between successive measurements well (Supporting Information Fig. A1f–h), the stepwise method (Fig. 5f) and stepwise method variant 2 (Table 1), for which we used measured DO to calculate DO saturation deficit and matched measured and modeled DO (Fig. 5h), fit the DO concentration trajectory poorly. Stepwise method variant 1 (Table 1), for which modeled DO was used to calculate DO saturation deficit, fit DO concentration trajectory well (Fig. 5g).

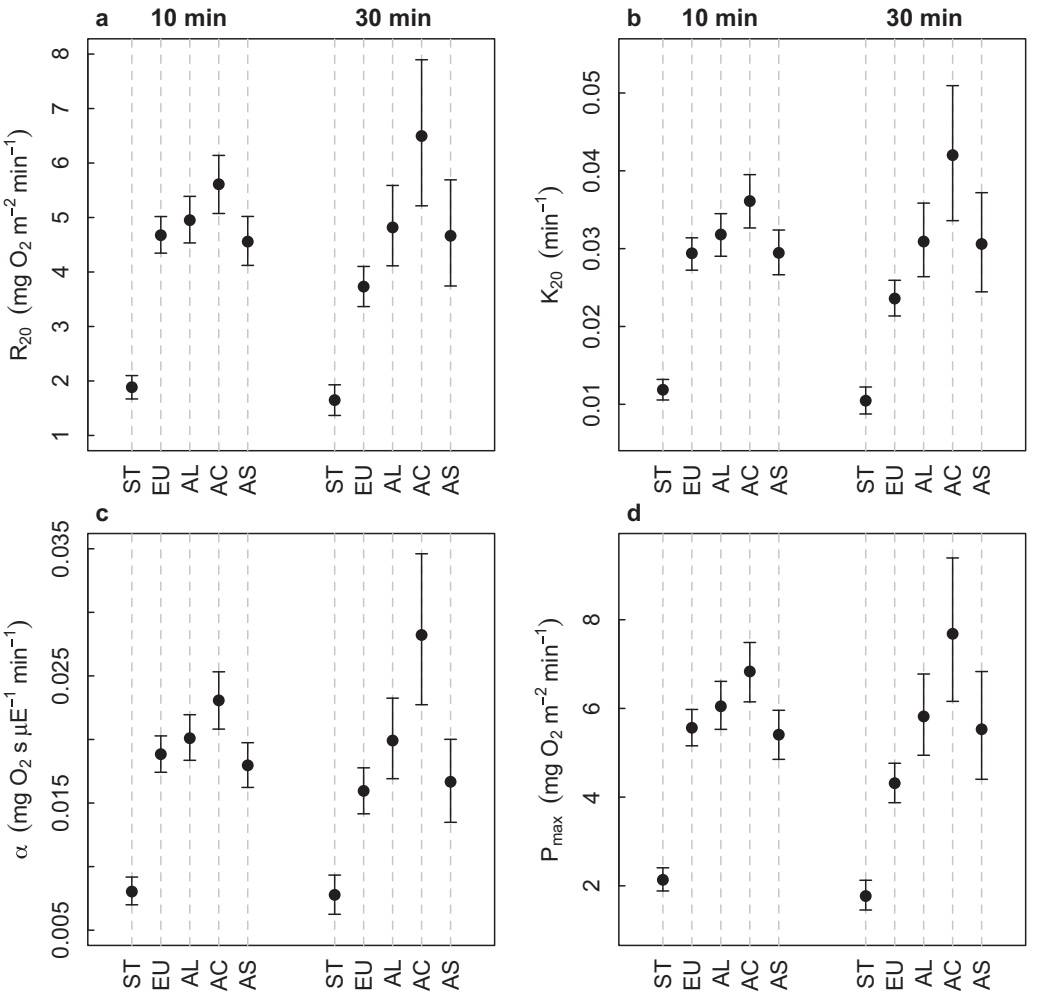

Fig. 3. Parameter estimates with different methods of numerically solving the DO differential equation and interpolating light and temperature: stepwise method (ST), Euler method (EU), accurate method with linear interpolation (AL), accurate method with piecewise constant interpolation (AC) and accurate method with smoothing spline interpolation (AS). The four panels show estimates of R_{20} (a), K_{20} (b), α (c) and P_{max} (d), respectively. In each panel, the left side shows the estimates based on data with 10 min logging interval and the right side shows the estimates based on data with 30 min logging interval. Points in the graph represent the posterior mean of parameters and the intervals are 95% highest posterior density intervals.

The Euler and accurate methods yielded much smaller magnitude of discrepancies in parameter (Fig. 3) and daily GPP and ER estimates (Fig. 4). However, the Euler method and the accurate method with piecewise constant interpolation resulted in significant differences in parameter and daily GPP and ER estimates, shown as non-overlapping confidence intervals (Figs. 3, 4, Supporting Information Tables A1, A2). In addition, the difference between the Euler method and the accurate method became more pronounced as the logging interval of DO increased (Figs. 3, 4). The modified Euler method by Hall et al. (2015) generated estimates much more consistent to those obtained using the accurate method than the basic Euler method (Supporting Information Table A4). The accurate, Euler and modified Euler methods by Hall et al. (2015) all fit the observed DO concentration (Fig. 5a–e) and DO changes between measurements well (Supporting Information Fig. A1a–e). The parameter and daily GPP and ER estimates obtained from stepwise, Euler and accurate methods with three interpolations of light and temperature are fully summarized in the appendix (see Supporting Information tables A1, A2 and A3).

Discussion

Generality of the comparison

Although we clearly demonstrated that different methods of solving the standard differential equation for DO dynamics (Eq. 1) and different means of interpolating light and temperature result in differences in metabolism estimates (Figs. 3, 4), our comparison is based on one representative data set. The DO data we used are from Kings Creek, a typical prairie stream that has been a model system for extensive studies of metabolism rates historically (Dodds et al. 1996;

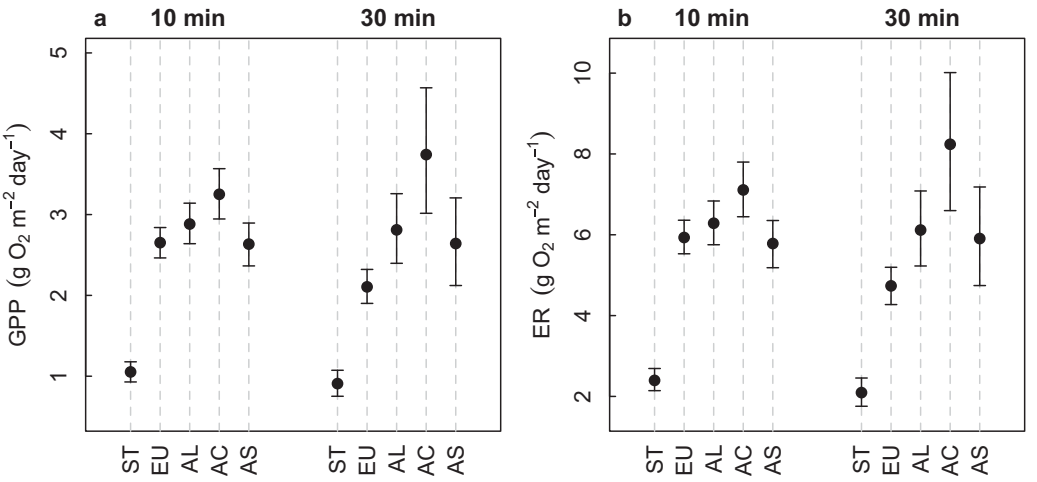

Fig. 4. Daily GPP (a) and ER (b) estimates with different methods of solving the DO differential equation and interpolating light and temperature: stepwise method (ST), Euler method (EU), accurate method with linear interpolation (AL), accurate method with piecewise constant interpolation (AC) and accurate method with smoothing spline interpolation (AS). In each panel, the left side shows the estimates based on data with 10 min logging interval and the right side shows the estimates based on data with 30 min logging interval. Points in the figure represent the posterior mean of daily GPP and ER, and the intervals represent 95% highest posterior density intervals.

Mulholland et al. 2001; Wilson and Dodds 2009; Bernot et al. 2010; Murdock et al. 2010; Riley and Dodds 2012). The daily GPP and ER rates in this stream from our estimates based on accurate and Euler methods, as well as previous estimates are in the range commonly found in headwater streams (Mulholland et al. 2001; Bernot et al. 2010). Thus, we imagine that the comparisons among methods made using this data set can be viewed as fairly general. However, without testing the methods using multiple data sets, we cannot definitively conclude that the particular magnitude and direction of differences found in this study will apply to all headwater streams. Therefore, our discussion focuses on the potential influences of different methods on metabolism estimates, not on whether these methods will always influence metabolism estimates in a particular way.

Stepwise method

We showed that the stepwise method significantly underestimated both the parameters and the daily GPP and ER rates. The particular direction and magnitude of differences found in this study are in agreement with previous work. Grace et al. (2015) found in an extensive data set that the daily GPP and ER estimates based on the stepwise method they implemented were highly correlated with but often lower than estimates based on the accurate numerical method implemented by Holtgrieve et al. (2010). Through the comparisons performed here, we demonstrated that such differences can arise due to the numerical method used to obtain a solution to the DO differential equation and the associated assumption about error distribution.

Stepwise, Euler and accurate methods with piecewise constant interpolation assume the same interpolation of light and temperature. Thus, the fact that the stepwise method resulted in dramatic differences in parameter estimates suggests that such difference was primarily the result of using measured DO to calculate DO saturation deficit or the result of the different assumption about error (Table 1). To determine the source of the differences, we implemented two variants of the stepwise method (Table 1). We found that parameter estimates based on both variants (Supporting Information Table A4) were quite different from those obtained from the Euler and accurate methods (Supporting Information Table A1). Thus, using measured DO to calculate DO saturation deficit or assuming independent and identically distributed normal error between modeled and measured changes in DO concentration $(\Delta[O_2]_{\text{measured},t} - \Delta[O_2]_{\text{modeled},t} \sim N(0, \sigma^2))$ can cause significant differences in parameter estimates. Therefore, it is necessary to evaluate and justify the assumptions before making a choice of computational method. Theoretically, we can examine the consistency between underlying assumptions and computation methods, and judge the validity of assumptions based on ecological understanding of the focal system. Statistically, the model fit to data may provide evidence in favor of or against a particular assumption, but it is worth remembering that model fit itself does not definitively prove or invalidate a particular error assumption. The poor fit could be a result of proper error assumption but an inappropriate formulation of GPP and ER. We thus argue that evidence from the examination of model fit should be viewed as suggestive.

The basic stepwise method uses measured DO to calculate DO saturation deficit instead of using modeled DO, which is inconsistent with the typical assumptions of observation error regarding differences between DO

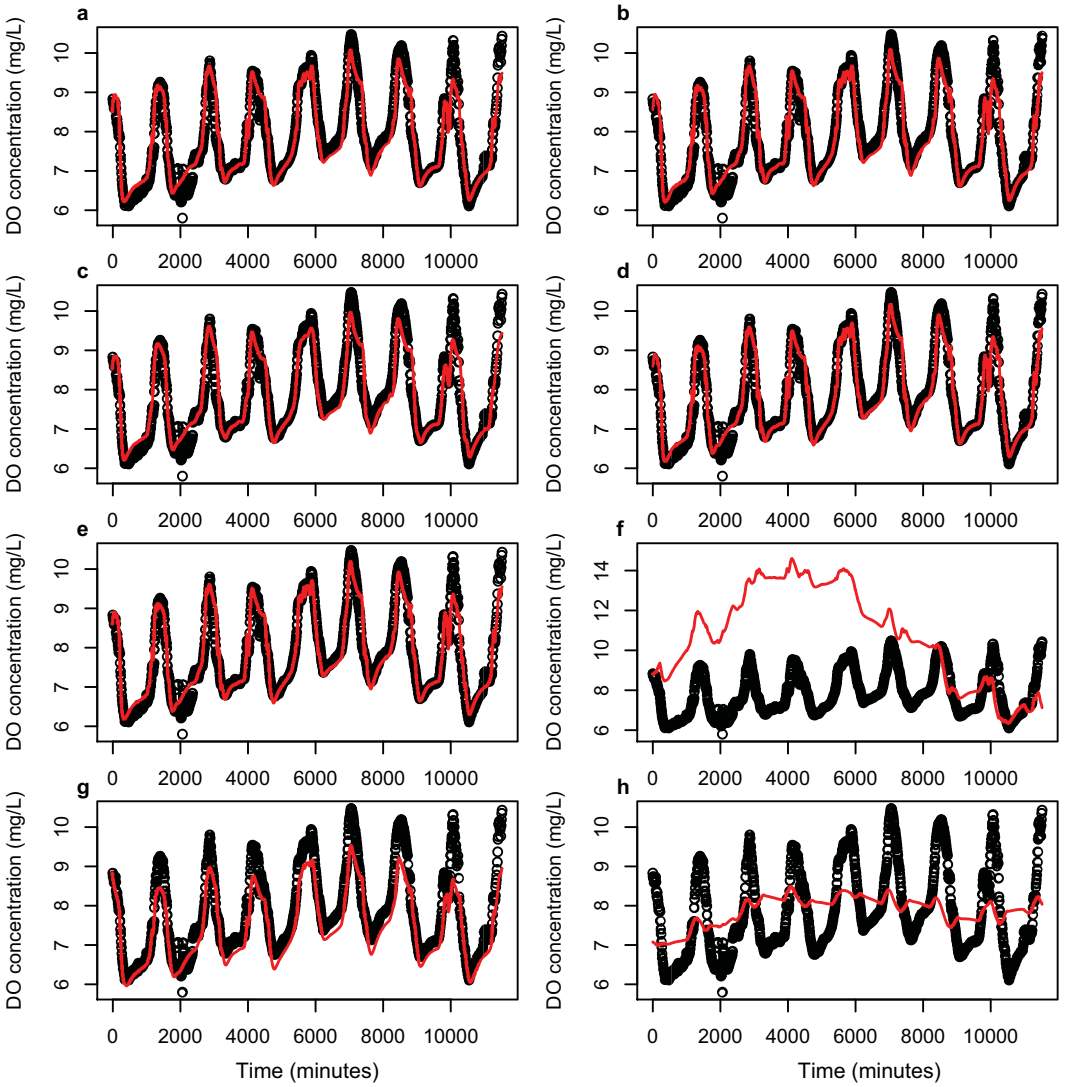

Fig. 5. Observed (dots) and modeled (red line) DO concentration for data with 10 min logging interval based on (a) accurate method with linear interpolation, (b) accurate method with piecewise constant interpolation, (c) accurate method with smoothing spline interpolation, (d) Euler method, (e) modified Euler method by Hall et al. (2015), (f) stepwise method, (g) stepwise method variant 1, using modeled DO in DO saturation deficit calculation and assuming independent and identically distributed normal error between measured and modeled DO changes, and (h) stepwise method variant 2, using measured DO in DO saturation deficit calculation and assuming independent and identically distributed normal error between measured and modeled DO concentration.

changes prescribed by Eq. 1 and observed DO changes between successive measurements. The assumption of observation error postulates that the model reflects the true average DO concentration given the "true" value of the parameters in Eq. 1 (Hilborn and Mangel 1997). Any deviation between modeled and measured DO concentration changes between successive measurements is the result of observation error, including inaccuracy of instruments or random deviation of DO concentration from the reach average in any specific parcel of water being measured. With such an assumption, it is clear that using modeled DO concentration to calculate reaeration is appropriate because the model reflects the true average DO concentration. Using measured DO to calculate reaeration is logically inconsistent with the assumption of observation error. For example, with an inappropriate set of parameters for Eq. 1, the modeled trajectory of DO will be very far from the measurement and this discrepancy will significantly influence the calculation of DO saturation deficit, as it should. It is this discrepancy that is critical for assessing or inferring the probability of a particular set of parameters. Therefore, if we use measured DO to calculate DO saturation deficit, we do not properly "penalize" the inappropriate set of parameters. This could be one of the reasons for the huge

discrepancy in metabolism estimates between the stepwise method and other methods.

Alternatively, one might assume a process error model for which the DO concentration is relatively uniform and DO measurements are error free. The measured DO then correctly reflects the true average DO concentration, and any discrepancy between measured and modeled DO would be due to processes unaccounted for in the model. In this situation, using measured DO to calculate DO saturation deficit would be appropriate. However, the assumption of independent and identically distributed normal process errors could be problematic. Any processes that change DO concentration are likely to be systematic and thus, it is unreasonable and unrealistic to assume that independent, identically distributed random deviations would be caused by such systematic processes. More importantly, such an assumption implies that the model does not fully capture the processes influencing DO dynamics. In this situation, simply using a method supported by an incomplete model is not the best remedy. The more appropriate remedy is to incorporate the ignored processes in the model although this may be quite difficult. For example, McCutchan et al. (2002) and Hall and Tank (2005) explicitly modeled groundwater input to account for its influence on DO concentration and on metabolism estimates.

Although using measured DO to calculate DO saturation deficit is theoretically consistent with a process error model, the stepwise method that makes the assumption of independent and identically distributed normal process error results in a model that fits DO changes well (Supporting Information Fig. A1f), but provides a very poor fit to the observed DO concentration data (Fig. 5f). Variant 2 of stepwise method (Table 1) also resulted in a poor fit to the observed DO concentration trajectory (Fig. 5h). This variant of the stepwise method and the Euler methods differ only in whether measured or modeled DO is used in the calculation of the DO saturation deficit (Table 1). Together, the relatively good fit of the Euler method (Fig. 5d) and the poor fit of the stepwise method (Fig. 5f) and stepwise method variant 2 (Fig. 5h) suggest that the assumption of independent and identically distributed normal process error is unlikely to be valid. This does not necessarily invalidate a process error model, but clearly illustrates that the distributional assumption of process error thus specified is inadequate, at least for our data set.

The dramatically different metabolism estimates obtained with the stepwise method could also result from fitting modeled changes in DO to data instead of fitting modeled DO concentration to data, assuming independent and identically distributed normal error between the measured and modeled changes in DO concentration ($\Delta[O_2]_{\text{measured},t} - \Delta[O_2]_{\text{modeled},t} \sim N(0, \sigma^2)$). Stepwise method variant 1 also underestimated the parameters and daily GPP and ER rates, although to much less of an extent compared to the variant 2 (Supporting Information Table A4). Variant 1 of the stepwise method differs from the Euler method only in that it fits modeled DO changes instead of modeled DO concentration to data (Table 1). This suggests that the different distributional assumption of error could also be responsible for the underestimation of parameters and daily GPP and ER. Variant 1 of the stepwise method resulted in a visually good fit to observed DO (Fig. 5g) and changes in DO (Supporting Information Fig. A1g) data. The apparent good fit of the stepwise method variant 1 (Fig. 5g, Supporting Information Fig. A1g) and the Euler method (Fig. 5d, Supporting Information Fig. A1d) suggest that either distributional assumption of error could be reasonable, but the fact that metabolism estimates differ between the two methods illustrates that apparently good fit alone is insufficient for guaranteeing accurate parameter and flux estimates.

Euler method

We demonstrated that the Euler method and the accurate method with different interpolation of light and temperature result in similar parameters and metabolism estimates that collectively differ from those generated by the stepwise method (Figs. 3, 4). However, the confidence intervals of parameter estimates and daily GPP and ER estimates between the Euler method and accurate method with piecewise constant interpolation do not overlap for both 10 min and 30 min logging intervals (Figs. 3, 4, Supporting Information Tables A1, A2). Because the Euler method only uses light and temperature at the measurement time, it is equivalent to a piecewise constant interpolation of light and temperature. Therefore, the difference in metabolism estimates between the Euler method and the accurate method with piecewise constant interpolation is purely due to the difference in how Eq. 1 is solved numerically. Specifically, the difference lies in whether changes in DO concentration during one logging interval are accounted for in the calculation of DO saturation deficit. Thus, the Euler approximation will likely result in larger differences in parameters estimates and in GPP and ER when DO concentration changes significantly on timescales shorter than the logging interval, and differences between the Euler and accurate methods will be more pronounced as the logging interval increases as we demonstrated in this study. Consequently, researchers should consider whether the difference caused by Euler methods with a particular logging interval is acceptable. However, it is difficult to articulate a general rule on the suitable logging frequency for Euler method. We recommend testing a subset of the data with both exact and Euler methods and examining whether the discrepancy is acceptable for the particular research question.

One advantage of the Euler method over the accurate method is its efficiency in computation. Solving Eq. 1 using the accurate method is computationally intensive, and processing a large amount of metabolism data will often require

powerful and dedicated computational resources. For example, on a single core of a 2.0 GHz Intel Core i7 4750HQ CPU, it takes 5 min and 32 s to evaluate 80,000 iterations of MCMC using the Euler method for our example data set (logged every 10 min for 8 d) and it takes the accurate method with linear interpolation 45 h and 12 min to perform the same calculation. The numerical differences in parameter estimates and daily GPP and ER estimates between the Euler and exact methods decrease with step size, but such differences can be significant as shown by the non-overlapping confidence intervals. If the statistical differences in parameter estimates or GPP and ER estimates are important for a specific research question, the Euler method is inadequate, but if such numerical differences in parameter estimates and GPP and ER estimates are tolerable in an ecological sense, the Euler method could be an acceptable compromise if the computational resources required for the accurate method are unavailable. Recently, Hall et al. (2015) modified the Euler method to include the average of modeled DO concentrations at the beginning and end of the logging interval in the calculation of DO saturation deficit. We used this method with 10 min logging interval data and obtained the parameter and mean daily GPP and ER estimates. Compared to the standard Euler method, this modification resulted in estimates more consistent with the values obtained using the accurate method with piecewise constant interpolation of light and temperature (Supporting Information Table A4). Although we are not aware of a strict mathematical proof of the convergence and stability of such a modified method of solving differential equation, the result from our study suggested that this method might provide a relatively accurate solution while maintaining the advantage of computation speed.

Influences of interpolation

We also compared how different methods of interpolating light and temperature influence metabolism estimates. Among the three methods compared in this study, the piecewise constant interpolation results in the greatest discrepancy in estimates compared to the linear and smoothing spline interpolations (Figs. 3, 4). One way to choose the most appropriate interpolation method would be to first interpolate the data with different methods based on subsampled data and then compare the interpolation with the actual measurements. Given the continuous nature of light and temperature, the linear interpolation and smoothing spline interpolation are more reasonable as they represent the continuous changes in light and temperature rather than the abrupt change at the end of a logging interval in the piecewise constant interpolation (Fig. 2a–c). However, rates of primary production and respiration may not respond to changes in light and temperature instantaneously. Due to the time lag of response, it is possible that the piecewise constant interpolation provides a better approximation given a particular combination of time lag of response and logging interval of light and temperature. Although piecewise constant interpolation may compensate for the time lag of responses, using a less realistic approximation to compensate for factors not included in the model is not an ideal approach. A better approach is to incorporate the time lag of response in the model of DO dynamics. In our study, the metabolism estimates based on linear and smoothing spline interpolations are very similar. Therefore, we conclude that either linear interpolation or smoothing spline interpolation are reasonable, and the choice of interpolation between these two methods is unlikely to cause significant differences in metabolism estimates.

Recommendation

The choice of computational methods involves both theoretical and practical considerations. The chosen method should be logically consistent with the underlying model assumptions and practically feasible for implementation. From a theoretical perspective, the stepwise method is a process error model and is not consistent with the assumption of observation error. The assumption of identically and independent distributed process error is unlikely to be ecologically realistic and resulted in a poor model fit with the data set used here. Using a model with inconsistent assumptions could lead to significant differences in parameter, GPP, and ER estimates. Therefore, we recommend that researchers carefully evaluate the model assumptions before applying the stepwise method.

The Euler method, although logically consistent with the assumptions of an observation error model, can lead to statistically significant differences in parameter and in GPP and ER estimates. Therefore, the accurate method is always preferred if we assume an observation error model. However, if computational resources are not available to implement the accurate method, and the error associated with Euler method is tolerable, the Euler method is an acceptable approach. Finally, we recommend using either linear or smoothing spline interpolations for light and temperature, and the choice between these two methods is unlikely to affect metabolism estimate in a significant way.

References

American Public Health Association. 1995. Standard methods for the examination of water and wastewater, 19th ed. American Public Health Association, American Water works Association and Water Environment Federation.

Bernot, M. J., and others. 2010. Inter-regional comparison of land-use effects on stream metabolism. Freshw. Biol. **55**: 1874–1890. doi:10.1111/j.1365-2427.2010.02422.x

Borges, A. V., B. Delille, L. S. Schiettecatte, F. Gazeau, G. Abril, and M. Frankignoulle. 2004. Gas transfer velocities of CO_2 in three European estuaries (Randers Fjord,

Scheldt, and Thames). Limnol. Oceanogr. **49**: 1630–1641. doi:10.4319/lo.2004.49.5.1630

Bott, T. L. 2006. Primary productivity and community respiration, p. 553–556. In E. R. Hauer and G. A. Lamberti [eds.], Methods in stream ecology. Academic Press.

Chapra, S. C., and D. M. Di Toro. 1991. Delta method for estimating primary production, respiration, and reaeration in streams. J. Environ. Eng. **117**: 640–655. doi:10.1061/(ASCE)0733-9372(1991)117:5(640)

Clark, J. F., H. J. Simpson, R. F. Bopp, and B. L. Deck. 1995. Dissolved oxygen in lower Hudson Estuary: 1978–93. J. Environ. Eng. **121**: 760–763. doi:10.1061/(ASCE)0733-9372(1995)121:10(760)

Cole, J. J., and N. F. Caraco. 1998. Atmospheric exchange of carbon dioxide in a low-wind oligotrophic lake measured by the addition of SF6. Limnol. Oceanogr. **43**: 647–656. doi:10.4319/lo.1998.43.4.0647

Crusius, J., and R. Wanninkhof. 2003. Gas transfer velocities measured at low wind speed over a lake. Limnol. Oceanogr. **48**: 1010–1017. doi:10.4319/lo.2003.48.3.1010

Demars, B. O. L., J. Thompson, and J. R. Manson. 2015. Stream metabolism and the open diel oxygen method: Principles, practice, and perspectives. Limnol. Oceanogr.: Methods **13**: 356–374. doi:10.1002/lom3.10030

Dodds, W. K., and others. 1996. The relationship of floods, drying, flow and light to primary production and producer biomass in a prairie stream. Hydrobiologia **333**: 151–159. doi:10.1007/BF00013429

Elmore, H. L., and W. F. West. 1961. Effect of water temperature on stream reaeration. J. Sanit. Eng. Div. **87**: 59–71.

Geweke, J. 1992. Evaluating the accuracy of sampling-based approaches to calculating posterior moments, p. 169–193. In J. M. Bernado, J. O. Berger, A. P. Dawid and A. F. M. Smith [eds.], Bayesian statistics 4. Clarendon Press.

Geyer, C. J., and L. T. Johnson. 2014. mcmc: Markov Chain Monte Carlo. R package version 0.9–3.

Grace, M. R., D. P. Giling, S. Hladyz, V. Caron, R. M. Thompson, and R. Mac Nally. 2015. Fast processing of diel oxygen curves: Estimating stream metabolism with BASE (BAyesian Single-station Estimation). Limnol. Oceanogr.: Methods **13**: 103–114. doi:10.1002/lom3.10011

Gulliver, J. S., and H. G. Stefan. 1984. Stream productivity analysis with dorm–I: Development of computational model. Water Res. **18**: 1569–1576. doi:10.1016/0043-1354(84)90132-5

Haario, H., E. Saksman, and J. Tamminen. 2001. An adaptive Metropolis algorithm. Bernoulli **7**: 223–242. doi:10.2307/3318737

Hall, R. O., and J. L. Tank. 2005. Correcting whole-stream estimates of metabolism for groundwater input. Limnol. Oceanogr.: Methods **3**: 222–229. doi:10.4319/lom.2005.3.222

Hall, R. O., J. L. Tank, M. A. Baker, E. J. Rosi-Marshall, and E. R. Hotchkiss. 2015. Metabolism, gas exchange, and carbon spiraling in rivers. Ecosystems **19**: 1–14. doi:10.1007/s10021-015-9918-1

Hanson, P. C., S. R. Carpenter, N. Kimura, C. Wu, S. P. Cornelius, and T. K. Kratz. 2008. Evaluation of metabolism models for free-water dissolved oxygen methods in lakes. Limnol. Oceanogr.: Methods **6**: 454–465. doi:10.4319/lom.2008.6.454

Hilborn, R., and M. Mangel. 1997. The ecological detective: Confronting models with data. Princeton Univ. Press.

Hindmarsh, A. C. 1983. ODEPACK, A systematized collection of ODE solvers, p. 55–64. In R. S. Stepleman and others [eds.], Scientific computing. North–Holland Publishing Company.

Holtgrieve, G. W., D. E. Schindler, T. A. Branch, and Z. T. A'Mar. 2010. Simultaneous quantification of aquatic ecosystem metabolism and reaeration using a Bayesian statistical model of oxygen dynamics. Limnol. Oceanogr. **55**: 1047–1063. doi:10.4319/lo.2010.55.3.1047

Holtgrieve, G. W., D. E. Schindler, and K. Jankowski. 2015. Comment on Demars et al. 2015, "Stream metabolism and the open diel oxygen method: Principles, practice, and perspectives". Limnol. Oceanogr.: Methods **14**: 110–113. doi:10.1002/lom3.10075

Hornberger, G. M., and M. G. Kelly. 1975. Atmospheric reaeration in a river using productivity analysis. J. Environ. Eng. Div. **101**: 729–739.

Hotchkiss, E. R., and J. R. O. Hall. 2014. High rates of daytime respiration in three streams: Use of $\delta^{18}O_{O2}$ and O_2 to model diel ecosystem metabolism. Limnol. Oceanogr. **59**: 798–810. doi:10.4319/lo.2014.59.3.0798

Jassby, A. D., and T. Platt. 1976. Mathematical formulation of the relationship between photosynthesis and light for phytoplankton. Limnol. Oceanogr. **21**: 540–547. doi:10.4319/lo.1976.21.4.0540

Jonsson, A., J. Åberg, A. Lindroth, and M. Jansson. 2008. Gas transfer rate and CO_2 flux between an unproductive lake and the atmosphere in northern Sweden. J. Geophys. Res. Biogeosci. **113**: G04006. doi:10.1029/2008jg000688

Kremer, J. N., A. Reischauer, and C. D'Avanzo. 2003. Estuary-specific variation in the air-water gas exchange coefficient for oxygen. Estuaries **26**: 829–836. doi:10.1007/BF02803341

Marino, R., and R. W. Howarth. 1993. Atmospheric oxygen exchange in the Hudson River: Dome measurements and comparison with other natural waters. Estuaries **16**: 433–445. doi:10.2307/1352591

Marzolf, E. R., P. J. Mulholland, and A. D. Steinman. 1994. Improvements to the diurnal upstream-downstream dissolved oxygen change technique for determining whole-stream metabolism in small streams. Can. J. Fish. Aquat. Sci. **51**: 1591–1599. doi:10.1139/f94-158

McCutchan, J., and others. 2002. Effects of groundwater flux on open-channel estimates of stream metabolism.

Limnol. Oceanogr. **47**: 321–324. doi:10.4319/lo.2002.47.1.0321

Megard, R. O., D. W. Tonkyn, and W. H. Senft. 1984. Kinetics of oxygenic photosynthesis in planktonic algae. J. Plankton Res. **6**: 325–337. doi:10.1093/plankt/6.2.325

Melching, C. S., and H. E. Flores. 1999. Reaeration equations derived from US Geological Survey database. J. Environ. Eng. **125**: 407–414. doi:10.1061/(ASCE)0733-9372(1999)125:5(407)

Mulholland, P. J., and others. 2001. Inter-biome comparison of factors controlling stream metabolism. Freshw. Biol. **46**: 1503–1517. doi:10.1046/j.1365-2427.2001.00773.x

Murdock, J. N., K. B. Gido, W. K. Dodds, K. N. Bertrand, and M. R. Whiles. 2010. Consumer return chronology alters recovery trajectory of stream ecosystem structure and function following drought. Ecology **91**: 1048–1062. doi:10.1890/08-2168.1

Odum, H. T. 1956. Primary production in flowing waters. Limnol. Oceanogr. **1**: 102–117. doi:10.4319/lo.1956.1.2.0102

Parkhill, K. L., and J. S. Gulliver. 1999. Modeling the effect of light on whole-stream respiration. Ecol. Model. **117**: 333–342. doi:10.1016/S0304-3800(99)00017-4

Petzold, L. 1983. Automatic selection of methods for solving stiff and nonstiff systems of ordinary differential equations. SIAM J. Sci. Stat. Comput. **4**: 136–148. doi:10.1137/0904010

Plummer, M., N. Best, K. Cowles, and K. Vines. 2006. CODA: Convergence diagnosis and output analysis for MCMC. R news **6**: 7–11.

R Core Team. 2015. R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria.

Raymond, P. A., and others. 2012. Scaling the gas transfer velocity and hydraulic geometry in streams and small rivers. Limnol. Oceanogr. Fluids Environ. **2**: 41–53. doi:10.1215/21573689-1597669

Reichert, P., U. Uehlinger, and V. Acuña. 2009. Estimating stream metabolism from oxygen concentrations: Effect of spatial heterogeneity. J. Geophys. Res. Biogeosci. **114**: G03016. doi:10.1029/2008jg000917

Riley, A. J., and W. K. Dodds. 2012. The expansion of woody riparian vegetation, and subsequent stream restoration, influences the metabolism of prairie streams. Freshw. Biol. **57**: 1138–1150. doi:10.1111/j.1365-2427.2012.02778.x

Riley, A. J., and W. K. Dodds. 2013. Whole-stream metabolism: Strategies for measuring and modeling diel trends of dissolved oxygen. Freshw. Sci. **32**: 56–69. doi:10.1899/12-058.1

Soetaert, K., T. Petzoldt, and R. W. Setzer. 2010. Solving differential equations in R: Package deSolve. J. Stat. Softw. **33**: 1–25. doi:10.18637/jss.v033.i09

Solomon, C. T., and others. 2013. Ecosystem respiration: Drivers of daily variability and background respiration in lakes around the globe. Limnol. Oceanogr. **58**: 849–866. doi:10.4319/lo.2013.58.3.0849

Tsivoglou, E. C., and L. A. Neal. 1976. Tracer measurement of reaeration: III. Predicting the reaeration capacity of inland streams. Journal (Water Pollution Control Federation) **48**: 2669–2689.

Van de Bogert, M. C., S. R. Carpenter, J. J. Cole, and M. L. Pace. 2007. Assessing pelagic and benthic metabolism using free water measurements. Limnol. Oceanogr.: Methods **5**: 145–155. doi:10.4319/lom.2007.5.145

Wanninkhof, R. 1992. Relationship between wind speed and gas exchange over the ocean. J. Geophy. Res. **97**: 7373–7382. doi:10.1029/92JC00188

Wilson, K. C., and W. K. Dodds. 2009. Centimeter-scale stream substratum heterogeneity and metabolic rates. Hydrobiologia **623**: 53–62. doi:10.1007/s10750-008-9647-y

Young, R. G., and A. D. Huryn. 1998. Comment: Improvements to the diurnal upstream-downstream dissolved oxygen change technique for determining whole-stream metabolism in small streams. Can. J. Fish. Aquat. Sci. **55**: 1784–1785. doi:10.1139/f98-052

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