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New methods for estimating components of lake metabolism based on free-water dissolved-oxygen dynamics

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ABSTRACT

Exchange of carbon between the biosphere and atmosphere is dominated by rates of photosynthetic CO_2 uptake and respiratory CO_2 release by aquatic and terrestrial ecosystems worldwide. Obtaining accurate estimates of these rates is therefore important. In lakes, the most common estimation method is based on a model of dissolved-oxygen (DO) dynamics and a corresponding time series of DO concentrations measured in freely moving lake water. O_2 production and consumption are inferred from changes in DO concentration, then converted to estimates of carbon uptake and release using photosynthetic and respiratory quotients. The traditional method of this type uses a simple accounting procedure to estimate daily gross primary production (*GPP*), total respiration (*R*), and net production (*NP*). Assuming that measured DO concentrations contain no error, it attempts to back-calculate *GPP*, *R*, and *NP* from an observed time series without using statistical techniques. This method produces valid estimates of *GPP* and the nighttime component of *R*, but it is unable to estimate the daytime component of *R* and hence cannot estimate *R* or *NP* for a complete dark–light cycle. To obtain estimates of these quantities, one must subjectively assume a value for daytime respiration. We present three new methods for estimating *GPP*, *R*, and *NP* that resolve this problem and also facilitate assessment of model adequacy. We illustrate use of the methods and compare their parameter estimates by applying them to monitoring data from Muskegon Lake, Michigan (USA).

1. Introduction

Ecosystem metabolism is composed of two of the most fundamental processes in the biosphere: production and respiration (Biddanda et al., 1994). Fluxes of carbon and oxygen driven by biospheric primary production and respiration constitute one of the largest mass movements of elements on Earth (Schlesinger, 1997). Asynchrony among these two complementary processes results in the observed daily, seasonal, and annual cycles of life, as well as associated flows of bioactive elements at local, regional, and global scales (Keeling et al., 1996). Consequently, the importance of accurately estimating rates of metabolism in Earth's many sub-ecosystems cannot be overemphasized.

The three main components of lake metabolism are gross primary production (*GPP*), total respiration (*R*), and net production (*NP*) (Fig. 1). *GPP* is the amount of inorganic carbon incorporated into new biomass by photosynthetic organisms over a specified period of time. This carbon is derived from CO_2 taken up from the environment, with most of the photosynthetic reactions involved also producing O_2. *R* is the total amount of existing biomass (as carbon) catabolized and released as CO_2 over the same period of time by all aerobic organisms, with a corresponding uptake of O_2 from the environment. *GPP* and *R* therefore reflect the major rates at which carbon is gained and lost by biological components of the lake ecosystem due to physiological activities of organisms. *NP* is the difference between *GPP* and *R* and therefore represents the net gain or loss of biomass (as carbon) over the same period of time to which *GPP* and *R* apply.

GPP, *R*, and *NP* are useful in characterizing a variety of integrative properties of aquatic ecosystems or ecosystem components, such as the relative degree of heterotrophy versus autotrophy (Odum, 1956; Cole et al., 2000; Hanson et al., 2003; Lovett et al., 2006), associations between lake metabolism, lake geometry, and catchment properties (Staehr et al., 2012a), broad features of community structure (Odum, 1956; del Giorgio et al., 1999), trophic states of lakes (del Giorgio and Peters, 1994), the relative contributions of allochthonous versus autochthonous carbon (Odum, 1956; del Giorgio et al., 1999), and the response of community function to perturbations (Uehlinger and Naegeli, 1998; Uehlinger, 2000). They are also useful in comparing overall ecosystem function in different lakes or streams (Bott et al., 1985; del Giorgio et al., 1999; Mulholland et al., 2001; Hanson et al., 2003).

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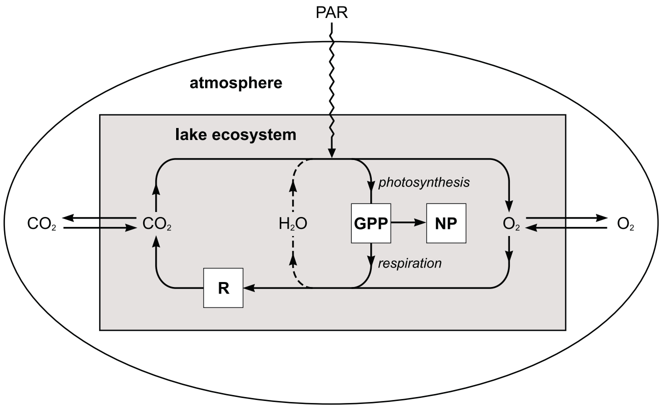

Fig. 1. Biological processes underlying the main components of lake metabolism. Oxygenic photoautotrophs use energy from photosynthetically active radiation (PAR) to produce biomass and oxygen (O_2) from water (H_2O), carbon dioxide (CO_2), and nutrients. The carbon content of biomass produced over a specified period of time is *gross primary production* (*GPP*). Some of the *GPP* is respired by aerobic organisms, producing CO_2 and H_2O and consuming O_2. The amount of carbon in CO_2 produced by respiration over the specified period of time is *total respiration* (*R*), and the residual amount of *GPP* not respired is *net production* (*NP*). The pools of dissolved CO_2 and O_2 in the lake also exchange with the atmosphere.

Obtaining estimates of *GPP*, *R*, and *NP* requires both an empirical method for obtaining the necessary data and a computational procedure for constructing the estimates. Various alternatives are available for carrying out each step, which we now briefly outline.

The first practical method for acquiring the necessary data in aquatic ecosystems was developed in the 1920s (light and dark bottle method: Gaarder and Gran, 1927). Several alternative techniques have been developed since then, with so-called free-water methods now being commonly used in stream and lake studies. All of these methods exploit the linkage between rates of gross primary production and total respiration on the one hand and rates of either CO_2 or O_2 uptake and release on the other (Cole et al., 2000; Bott, 2006; Hall et al., 2007; Staehr et al., 2010, 2012c). In this paper, we focus on the free-water dissolved-oxygen (DO) method as applied to lakes. This method entails deploying sensors in freely moving water to acquire high-frequency time-series data on DO concentration, water temperature, photosynthetically active radiation (PAR), and optionally other variables. A corresponding time series of weather data on wind speed and atmospheric pressure is also required. Carbon uptake and loss are inferred from DO dynamics by exploiting the roughly constant ratios of photosynthetic O_2 production to CO_2 consumption (photosynthetic quotient) and respiratory CO_2 production to O_2 consumption (respiratory quotient).

The acquired lake and weather data are used to estimate *GPP*, *R*, and *NP* by one of several alternative approaches. The most common one is based on a simple accounting procedure and an assumed value for daytime respiration. We will call this the accounting approach. It was developed by Sargent and Austin (1949, 1954) and subsequently refined by Odum (1956). A much newer class of approaches employs process-based models of DO dynamics to predict time series of DO concentrations from observed times series of various lake and weather variables (Van de Bogert et al., 2007; Ciavatta et al., 2008; Hanson et al., 2008; Soetaert and Gregoire, 2011; Batt and Carpenter, 2012). We will call these prediction approaches. Estimates of *GPP*, *R*, and *NP* are obtained by integrating the appropriate terms of the fitted model over the time period of interest (e.g., one day).

The main purpose of the present paper is to derive three new prediction approaches to estimating *GPP*, *R*, and *NP*. We begin by constructing a continuous-time model of DO dynamics that underlies both the accounting and prediction approaches. We then derive the accounting approach and three prediction approaches within this common framework. For the accounting approach, we show how to derive the usual estimates of *GPP*, *R*, and *NP* so the required assumptions are clearly revealed. For the prediction approaches, we construct appropriate models that include an error component, show how to use these models to obtain least-squares estimates of parameter values, and show how to estimate *GPP*, *R*, and *NP* from the fitted models. We also illustrate and compare the accounting and prediction approaches by applying them to real data from a monitoring buoy in Muskegon Lake, Michigan, a tributary ecosystem to Lake Michigan.

2. The basic model of dissolved-oxygen dynamics

The starting point for free-water methods of estimating *GPP*, *R*, and *NP* in lakes is a mass-balance model of DO dynamics. In engineering studies of water quality in lakes and reservoirs, it has long been customary to conceptualize the production, consumption, and transport of DO as a continuum transport process. To make the models practical in applications, a single spatial dimension (vertical) typically is used. We briefly review this modeling framework (loosely following Bella, 1970), since it represents the main processes governing DO dynamics in a clear and natural way. We then show how to obtain the type of model typically used in ecological studies of lake metabolism by specializing the continuum transport framework.

Consider a vertical column of water, rectangular in horizontal cross-section and extending from the lake surface down to the bed (Fig. 2A). Let the horizontal cross-sectional area of the column of water be A, which is constant over depth and time. Throughout this paper, we refer to this column of water simply as the water column. In applications, a string of sensors will run vertically through the center of the water column, and we assume the values of DO concentration and other parameters measured at each depth hold for the entire horizontal slice of the column at that depth. We do not assume these values can be extrapolated to the entire lake.

The main physical processes that add, remove, and transport DO in lakes are summarized in Fig. 3. Given adequate PAR, photosynthetic bacteria and eukaryotic algae convert CO_2 and H_2O to O_2 and simple carbohydrates $[(CH_2O)_n]$, which are then used to synthesize other macromolecular components of biomass. All aerobic organisms in the lake remove DO through respiration. Flux of O_2 gas across the water surface occurs and can be positive (increasing DO concentration in near-surface lake water) or negative, depending on whether the current concentration of DO just beneath the water surface is below or above the current air–water equilibrium concentration. Exchange of O_2 also occurs across the other “walls” of the water column, due to various physical processes including advection, convection, and molecular and turbulent diffusion.

Let z represent distance below the water surface, with $z = 0$ corresponding to the surface and $z = D$ to the bed (Fig. 2A), and let z_1 and z_2 ($0 < z_1 < z_2 < D$) be two arbitrary depths in the water column. A simple mass-balance argument applied to the segment of the water column between z_1 and z_2 yields the following verbal equation, which integrates the effects of the various processes adding and removing DO:

$$\begin{bmatrix}\text{rate of}\\\text{change in}\\\text{DO mass}\end{bmatrix} = \begin{bmatrix}\text{rate of}\\\text{photosynthetic}\\\text{DO production}\end{bmatrix} - \begin{bmatrix}\text{rate of}\\\text{respiratory DO}\\\text{consumption}\end{bmatrix} + \begin{bmatrix}\text{rate of}\\\text{DO gain from}\\\text{vertical flux}\end{bmatrix} + \begin{bmatrix}\text{rate of}\\\text{DO gain from}\\\text{horizontal flux}\end{bmatrix} \tag{1}$$