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Impact of non-idealities in gas-tracer tests on the estimation of reaeration, respiration, and photosynthesis rates in streams

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ABSTRACT

Estimating respiration and photosynthesis rates in streams usually requires good knowledge of reaeration at the given locations. For this purpose, gas-tracer tests can be conducted, and reaeration rate coefficients are determined from the decrease in gas concentration along the river stretch. The typical procedure for analysis of such tests is based on simplifying assumptions, as it neglects dispersion altogether and does not consider possible fluctuations and trends in the input signal. We mathematically derive the influence of these non-idealities on estimated reaeration rates and how they are propagated onto the evaluation of aerobic respiration and photosynthesis rates from oxygen monitoring. We apply the approach to field data obtained from a gas-tracer test using propane in a second-order stream in Southwest Germany. We calculate the reaeration rate coefficients accounting for dispersion as well as trends and uncertainty in the input signals and compare them to the standard approach. We show that neglecting dispersion significantly underestimates reaeration, and results between sections cannot be compared if trends in the input signal of the gas tracer are disregarded. Using time series of dissolved oxygen and the various estimates of reaeration, we infer respiration and photosynthesis rates for the same stream section, demonstrating that the bias and uncertainty of reaeration using the different approaches significantly affects the calculation of metabolic rates.

1. Introduction

The variation of dissolved oxygen (DO) in streams is caused by several processes, of which respiration and primary production are considered to be the most important ones (Odum, 1956; Staehr et al., 2012). During respiration, DO is consumed by aerobic metabolism, whereas primary production leads to an increase of DO in the stream by photosynthesis. As such, both respiration and primary production provide information concerning the vitality and health of the ecosystem (Fellows et al., 2006; Young et al., 2008). The net ecosystem productivity is the difference between respiration and gross primary production and thus denotes the metabolism of a stream. It is usually measured either with the help of in-stream respiration chambers (McIntire et al., 1964; Uzarski et al., 2001) or via the open-water exchange method (Hoellein et al., 2013; Odum, 1956) based on oxygen measurements at one or two stations. Chamber measurements rely on recirculating water around a substrate sample, enabling controlled and replicable measurements. However, artifacts may be caused by non-representative sampling, community disruption and unnatural environments (Bothwell, 1985, 1988, 1989; Horner et al., 1990) preventing upscaling of the results to the whole stream (Bott et al., 2006; Marzolf et al., 1994). The open-water exchange method on the other hand determines metabolic rates from diurnal changes of dissolved-oxygen concentrations. As such, it integrates metabolism over the studied reach and is performed in a natural, undisturbed environment. However, this approach can only be applied where groundwater inflow is negligible (Marzolf et al., 1994; Tank et al., 2010). Furthermore, an independent measurement of reaeration is required in order to determine metabolism rates from oxygen data.

Reaeration changes the DO concentration in the stream towards the saturation concentration, describing the equilibrium with the atmosphere. In case of under-saturation, oxygen is introduced into

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the stream by reaeration, but if the stream is over-saturated, oxygen is lost to the atmosphere by the same process. The direction and magnitude of this process is thus highly variable and for accurately calculating metabolic turnover rates, an accurate estimation of reaeration rates is vital. These reaeration rate coefficients, however, are difficult to determine, as all known approaches suffer from inherent shortcomings: Expressions approximating reaeration coefficients from readily available stream data, such as discharge, water depth, and bottom slope, are only applicable under very specific conditions and outcomes calculated by different expressions may differ greatly (Bennett and Rathbun, 1972). Methods relying on longitudinal DO-profiles (e.g., Odum, 1956) are often biased, especially if influenced by varying temperature and nonlinear photosynthesis effects (Kosinski, 1984). According to Marzolf et al. (1994) and Wanninkhof et al. (1990), the determination of reaeration coefficients by gas-tracer tests is the most reliable method. In this approach, a volatile compound is continuously injected into the stream and its concentration is measured at one or more downstream locations after steady-state conditions have been reached. From the observed decrease in tracer concentrations along the reach, the reaeration rate coefficient can be directly determined. Propane has frequently been applied as gas tracer (e.g., Marzolf et al., 1994; Young and Huryn, 1999), because the reaeration rate coefficients obtained for this compound can easily be transferred to those of oxygen due to similar Henry's law and molecular diffusion coefficients (Rathbun et al., 1978).

Thus, gas-tracer tests have become a standard evaluation tool for the assessment of oxygen cycling in streams, and the analysis as described by Genereux and Hemond (1990) and Wanninkhof et al. (1990), among others, is relatively simple and easy to implement. Unfortunately, the standard approach is also based on a series of simplifying assumptions that are often not questioned: (i) transport is considered to be strictly advective which, as we will show, leads to systematic underestimation of the reaeration coefficient, (ii) the input of the gas tracer must be steady, which is difficult to achieve with standard field equipment, (iii) if a temperature correction is applied, a constant temperature is assumed over the course of the experiment, (iv) a rigorous uncertainty analysis is typically missing.

The aims of this paper are: (1) to assess the impact of dispersion, unsteady input signals, and temperature changes on the estimation of reaeration rate coefficients and metabolic rates from gas-tracer tests, (2) to quantify the uncertainty of the estimated reaeration rate coefficient and its propagation to respiration and photosynthesis rates when conducting and analyzing gas-tracer tests, and (3) to suggest improvements for the calculation of reaeration rate coefficients from gas-tracer tests at different levels of complexity. Towards this end, we conducted a propane gas-tracer test in a small stream in Southwest Germany, sampling propane concentrations at four measurement stations. To investigate the stability of the propane signal, we conducted repeated sampling at the first station. From the break-through curves (BTCs) of a concurrent conservative-tracer test using fluorescein, we obtained complete travel time distributions as well as characteristic moments of the distributions for the individual sections.

We present analyses of the data according to different methods with increasing complexity to determine the impact of dispersion and an unsteady input signal on the estimation of reaeration rate coefficients in comparison to the standard approach. The uncertainty analysis is based on an ensemble approach applied to both travel time and the propane concentration with 5000 realizations. To show the effect of the different approaches on the calculation of metabolic rates, we used measured time series of DO and temperature to obtain respiration and photosynthesis rates for the different distributions of reaeration rate coefficients.

2. Theory

2.1. Estimation of reaeration rate coefficient

We consider linear transport of compounds in a stream with steady-state flow. The BTC $c_i^{down}(t)$ [ML^{-3}] of compound i at a downstream location can be computed from that at an upstream location $c_i^{up}(t)$ [ML^{-3}] by convolution with the transfer function $g_i(\tau)$ [T^{-1}]:

$$c_i^{down}(t) = \int_0^\infty g_i(\tau) c_i^{up}(t-\tau) d\tau \tag{1}$$

in which τ [T] is the travel time. The transfer function $g_i(\tau)$, also denoted unit-response function, is identical to the breakthrough curve at the downstream location for a pulse injection, multiplied with the discharge at the upstream location and divided by the injected mass. The transfer function between two stations downstream of an injection point can also be inferred from the corresponding measured BTCs by deconvolution without relying on a particular functional shape (Cirpka et al., 2007; Payn et al., 2008). In the following, we will denote the transfer function of a non-volatile, conservative compound $g(\tau)$ (without index), and that of a gas tracer $h(\tau)$, where we assume that the saturation concentration of the gas tracer is zero. The integral $R = \int_0^\infty g(\tau)d\tau \le 1$ [−] is the recovery of the conservative tracer, indicating dilution by lateral inflow over the stretch of the stream.

The normalized transfer function of the conservative tracer is the travel time distribution $p(\tau) = g(\tau)/R$ between the up- and downstream stations. If we assume Fickian, advective-dispersive transport with uniform coefficients, $p(\tau)$ is the inverse Gaussian distribution with the mean and standard deviation of travel time $\mu_\tau = x/v$ and $\sigma_\tau = \sqrt{2Dx/v^3}$, respectively (Kreft and Zuber, 1978), in which v [LT^{-1}] is the in-stream velocity, D [L^{2}T^{-1}] is the dispersion coefficient, and x [L] denotes the distance. At many streams, however, deviations from Fickian dispersion, notably extended tailing, have been observed (Cheong and Seo, 2003; Hunt, 1999).

If we follow a water parcel, the concentration c_g of a gas tracer with saturation concentration of zero undergoes linear loss to the atmosphere:

$$\frac{dc_g}{dt} = -k_2 c_g \tag{2}$$

with the gas-exchange or reaeration rate coefficient k_2 [T^{-1}]. From this, we can follow that the transfer function $h(\tau)$ of the gas tracer is:

$$h(\tau) = g(\tau)\exp(-k_2\tau) \tag{3}$$

If $g(\tau)$ is known from conservative-tracer BTCs, the reaeration rate coefficient k_2 can be estimated from up- and downstream concentrations $c_g^{up}(t)$ and $c_g^{down}(t)$ of the gas tracer by substituting Eq. (3) into Eq. (1) and fitting the resulting expression to $c_g^{down}(t)$.

In the standard approach to evaluate the reaeration rate coefficient, the inflow concentration $c_g^{up}(t)$ is assumed constant so that it can be factored out of the integral in Eq. (1). Also, rather than assuming a travel-time distribution, a single value is assumed. This yields after some rearrangement (Wanninkhof et al., 1990):

$$k_2 = \frac{1}{\mu_{\tau_{down}} - \mu_{\tau_{up}}} \ln\left(R\frac{c_g^{up}}{c_g^{down}}\right) \tag{4}$$

in which $\mu_{\tau_{up}}$ [T] and $\mu_{\tau_{down}}$ [T] denote the mean travel times