

Uncertainty in the estimation of stream metabolism from open-channel oxygen concentrations

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Abstract. The open-channel oxygen method for estimating stream metabolism avoids many of the problems associated with chamber techniques, but its uncertainty has not been rigorously quantified. Uncertainty in open-channel estimates of photosynthesis (P) and respiration (R) can be estimated by use of a Monte Carlo approach incorporating uncertainty in each of the terms (reaeration rate coefficient, range of temperature oscillation, midpoint temperature, travel time, metabolic rate, and precision of instrument calibration) affecting error in estimates of P and R. The distributions derived from the Monte Carlo simulations provide confidence limits for estimates of P and R. Use of this approach along with simulation of a range of stream conditions indicates that: 1) given equivalent metabolic rates and physical conditions, estimates of R are subject to greater uncertainty than are estimates of P, especially in high-gradient streams, and 2) uncertainty can be minimized by special attention to the precision of measurement for factors affecting the saturation concentration of oxygen. Reasonable confidence limits (95% CL within 30% of mean) can be achieved for estimates of P where daily photosynthetic rates exceed 4 mg L⁻¹d⁻¹, but in turbulent streams ($k_{20^{\circ}} = 100/d$), rates of R must be nearly 15 mg L⁻¹d⁻¹ to achieve similar precision.

Key words: stream metabolism, precision, error, photosynthesis, respiration, reaeration, Monte Carlo analysis.

Oxygen mass-balance techniques have been used to estimate stream metabolism in open channels (Odum 1956) and in recirculating chambers (e.g., Pennak and Lavelle 1979, Bott et al. 1985). The open-channel method offers several advantages over chambers because chambers may fail to account for the spatial heterogeneity of metabolism in streams and can introduce various chamber effects (Horner and Welch 1981, Marzolf et al. 1994). Unlike chamber techniques, the open-channel method rarely has been used in high-gradient streams because of difficulties in accounting for exchange of oxygen between the atmosphere and water where exchange rates are high. Recent improvements in methods for estimating gas exchange and the development of high-precision recording field meters have, however, made the measurement of metabolism in turbulent streams more feasible (Marzolf et al. 1994). Although the precision of reaeration estimates has been explored (Yotsukura et al. 1983, Kosinski 1984), uncertainty in final estimates of photosynthesis (P) and respiration (R) has not yet been examined rigorously.

The open-channel method depends on the measurement of deviations in stream oxygen concentration from saturation. Variations in con-

centration that cannot be explained by physical factors are attributed to biological processes. Application of the method requires measurements of dissolved oxygen, temperature, barometric pressure, and reaeration rate (exchange of oxygen with the atmosphere). Error in the measurement of each of these variables contributes to uncertainty in the final estimates of P and R. If the variance associated with each measurement can be characterized, a Monte Carlo approach can be used to determine the overall uncertainty in estimates of P and R, even if the frequency distributions of error in P and R are unknown beforehand (Law and Kelton 1991).

The purposes of this paper are to describe a simple method for estimating the uncertainty of stream metabolism measurements, to demonstrate how this method can be used to determine the suitability of the open-channel method to a particular location, and to show examples of uncertainty for a range of field conditions. The technique described here relies on commercially available software (@Risk, Pallisade Corporation, Newfield, NY) that samples randomly and repeatedly from the distribution that best characterizes the mean and variance of each variable contributing to error in the estimation of metabolic rates. The parameters considered here include the reaeration rate coefficient, travel

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time as it applies to estimation of the reaeration rate coefficient, the daily pattern of stream temperature oscillation, and the precision of instrument calibration.

Methods

The Monte Carlo approach as applied here assumes that each parameter contributing to an estimate of P and R corresponds to a random variable with an expected value equal to the true mean and with a normal frequency distribution (i.e., there is negligible bias in the mean of repeated measurements). A computer spreadsheet model is used to predict stream metabolism over a range of conditions. For each set of conditions, the Monte Carlo approach is used in the estimation of confidence limits (CL) for P and R given certain assumptions about the precision of measurements (i.e., variance in repeated measurements for a given set of conditions). The spreadsheet model thus permits the exploration of uncertainty over a wide range of stream conditions. Random sampling associated with the Monte Carlo approach was repeated until the means for estimated metabolic rates were within $0.01 \text{ mg O}_2 \text{ L}^{-1} \text{ d}^{-1}$ of expected rates.

Computer spreadsheet model

Under conditions of constant barometric pressure and with no accrual of water, the oxygen concentration at time t (C_t) for a homogeneous system can be approximated from the initial concentration (C_0), the reaeration coefficient for oxygen at temperature T ($k_{\text{Oxygen},T}$), the initial saturation deficit (D_0), processes that produce (P) or consume (R) oxygen, and the time between measurements (Δt) as follows:

$$C_t = C_0 + k_{\text{Oxygen}} D_0 \Delta t + (P - R) \Delta t \quad [1]$$

Temperature plays a central role in determining changes in oxygen concentration because it affects all physical and biological processes governing dissolved oxygen. In addition, temperature oscillates on a diel cycle and this oscillation can be large in small streams. Although temperature oscillation is sometimes described with a sine function for simplicity (e.g., Saunders et al. 1993), the diel oscillation is usually asymmetrical in streams and rivers less than 7th order (e.g., Kosinski 1984, Butcher and Covington 1995). We find for Colorado streams and rivers

that temperature is best represented by 2 equations: increasing temperature between sunrise and maximum daily temperature is represented by a sine function, and subsequently decreasing temperature is represented by logarithmic decay of temperature (J. McCutchan, unpublished data). For present purposes we use this 2-equation approach, by which the daily pattern of temperature can be predicted from 1) the length of time over which temperature increases, 2) the minimum temperature, and 3) the maximum temperature. The time at which maximum temperature occurs is typically 2/3 of the time between sunrise and sunset.

Light intensity (I) is a primary control over P and can be modeled with a 2-part equation (Chapra and Di Toro 1991). For a given maximum irradiance (I_{max}) and half-saturation irradiance (I_k), P can be adjusted for temperature and light intensity from a maximum rate at 20°C (Jassby and Platt 1976):

$$P_{\text{max},T} = P_{\text{max},20^\circ} \theta^{(T-20)} \quad [2]$$

$$P = P_{\text{max},T} \cdot \tanh\left(\frac{1}{I_k}\right) \quad [3]$$

For a Q_{10} of 2.0, the value of θ in equation 2 is set to 1.072. Respiration is scaled from a rate at 20°C using an equation of the same form as equation 2 ($\theta = 1.072$) and reaeration rate is scaled similarly ($\theta = 1.024$: Kilpatrick et al. 1989).

The computer spreadsheet model was used to predict changes in stream temperature and dissolved oxygen at 15-min intervals over a range of values for T_{mid} , $k_{\text{Oxygen},20^\circ}$, P_d (daily gross photosynthesis), and R_d (daily respiration). Unless otherwise specified, T_{mid} was set to 10°C , ΔT was set to 2.5°C , and P_d and R_d were set to $10 \text{ mg O}_2 \text{ L}^{-1} \text{ d}^{-1}$. Barometric pressure was set to 760 mm Hg, sunrise to 0600, and daylength to 12 h. I_k was set to $250 \mu\text{mol m}^{-2} \text{ s}^{-1}$ and I_{max} was set to $750 \mu\text{mol m}^{-2} \text{ s}^{-1}$.

Distributions of error for variables

The standard deviation (SD) for each random variable except for dissolved oxygen was determined empirically from multiple calibrations of equipment against certified instruments or from the literature (Table 1). The SD for measurements of dissolved oxygen was estimated empirically from 48-h continuous records of oxy-

TABLE 1. Characterization of error for variables used in estimation of metabolic rates. Standard deviations (SD) were determined empirically or from published values.

Measurement	SD	Resolution	Source
Temperature	0.05°C	0.01°C	a
Barometric pressure	0.6 mm Hg	1 mm Hg	a
Dissolved oxygen	0.01 mg/L	0.01 mg/L	b
Propane concentration (mean at each station)	0.5 ppb + 1.5% of measured concentration	0.1 ppb	b
Discharge	5% of measured discharge	N/A	c

^a J. McCutchan and R. Hamilton, unpublished data

^b J. McCutchan and L. Baumgartner, unpublished data

^c Yotsukura et al. 1983, McMahon and Bohlke 1996

gen concentration in a calibration chamber. The SD was set to ½ the maximum difference of that record from the mean.

All variables necessary to calculate metabolism are subject to a finite resolution, equal to the smallest unit of measure for a given instrument. Where reaeration rates are high, large metabolic rates result in only small deviations in stream oxygen concentrations. Rounding errors resulting from finite resolution of measurement thus can add to uncertainty in metabolism estimates. For modeling purposes, all measurements were rounded according to resolution values typical of instruments that are commonly used in metabolism studies (Table 1).

Volatile tracers such as propane (Kilpatrick et al. 1989) provide the most precise method for estimating the reaeration rate coefficient and are less prone to bias than are estimates based on physical characteristics (Marzolf et al. 1994). In their assessment of the propane technique, Yotsukura et al. (1983) quantify uncertainty in estimates of $k_{\text{Propane}20^\circ}$. A modification of their equation, which was determined by standard techniques for compounding errors, is used here to describe the variance associated with estimation of $k_{\text{Oxygen}20^\circ}$:

$$\sigma(k_{\text{Oxygen}20^\circ}) = \frac{1.39}{t_w} \sqrt{\frac{\sigma^2(C_u)}{n_{C_u}(\bar{C}_u)^2} + \frac{\sigma^2(C_d)}{n_{C_d}(\bar{C}_d)^2} + 2\frac{\sigma^2(Q)}{(Q)^2}} \quad [4]$$

where Q is discharge, C_u and C_d are the upstream and downstream propane concentrations, t_w is the water travel time between sampling stations, n is the number of measurements of propane concentration, and 1.39 is a conversion factor relating $k_{\text{Oxygen}20^\circ}$ to $k_{\text{Propane}20^\circ}$ (Kilpatrick et al. 1989). When travel time for propane

is set to $1/k_{\text{Oxygen}20^\circ}$ the change in propane concentration between sampling stations is constant and the SD for estimates of $k_{\text{Oxygen}20^\circ}$ is proportional to $k_{\text{Oxygen}20^\circ}$. Thus, uncertainty in estimates of $k_{\text{Oxygen}20^\circ}$ is greater at high than at low reaeration rates. This approach is more realistic than use of a fixed travel time because rapid tracer loss imposes a practical limit on travel times for propane in turbulent streams. For all simulations, discharge was set to $0.2 \text{ m}^3/\text{s}$, upstream propane concentration was set to 30 ppb, and 5 measurements of propane concentration were assumed for each station.

Estimates of uncertainty in P and R

From each simulated set of measurements, estimates of P and R were calculated by Odum's (1956) 2-station rate of change method, and error was estimated by the Monte Carlo method. Although the predicted rate of change curves for each set of measurements were identical, measurement errors for the upstream and downstream curves were computed separately. For each Monte Carlo iteration, errors in estimation of P and R were determined by the differences between rate of change curves incorporating variance and the rate of change curves calculated from the true dissolved oxygen and temperature values. The 95% CL for P and R were then determined from the distributions of error for simulated measurements of P and R . Metabolic rates and associated uncertainties are expressed in units of $\text{mg O}_2 \text{ L}^{-1} \text{ d}^{-1}$ to maintain generality in terms of stream depth. Conversion to areal values ($\text{mg O}_2 \text{ m}^{-2} \text{ d}^{-1}$) is accomplished by multiplying rates or errors by $1000 z_m/n_v$ where z_m is mean channel depth in m.

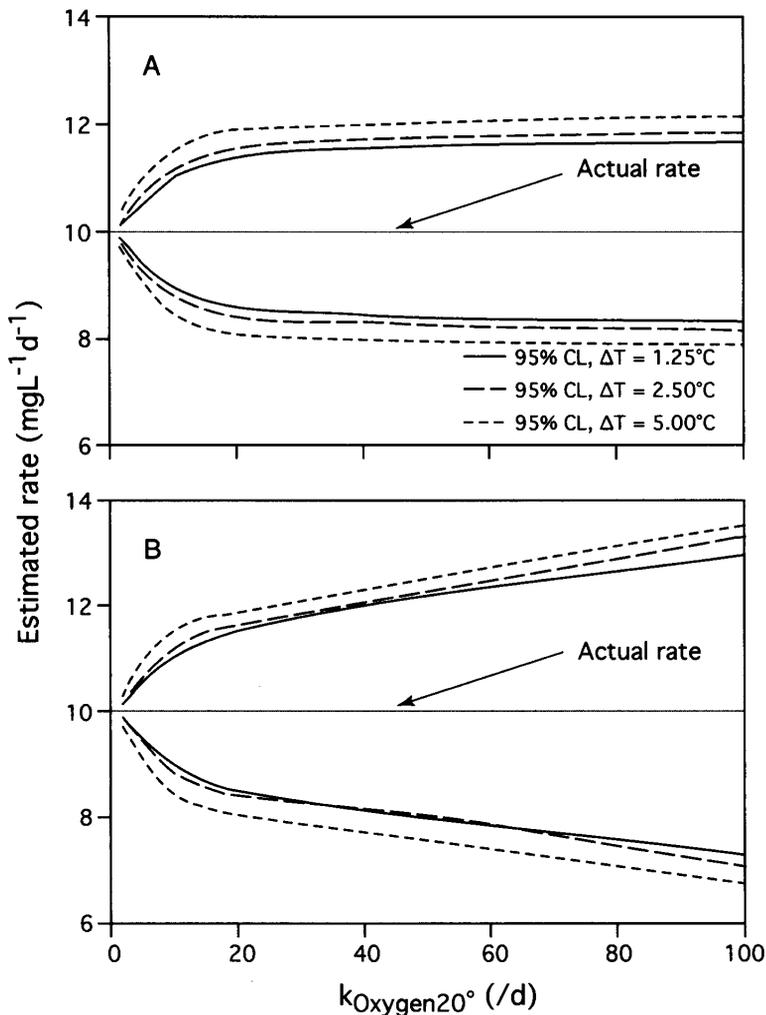


FIG. 1. Effects of range of temperature oscillation (ΔT) on 95% confidence limits (CL) for (A) photosynthesis and (B) respiration.

Results

The magnitude of the reaeration rate exerts a strong influence on uncertainty in estimates of metabolism. Where reaeration rates are very low (approximating chamber conditions), uncertainty in metabolism estimates is close to 0. Relative uncertainty (the magnitude of possible error as a fraction of the mean rate of metabolism) for estimates of P increases with increasing k_{20° (Figs. 1–3), but is approximately constant where $k_{\text{Oxygen}20^\circ}$ is $>20/\text{d}$. For estimates of R, uncertainty continues to increase with increasing $k_{\text{Oxygen}20^\circ}$ because calibration errors affect estimates of R more strongly than estimates of P. The ampli-

tude (ΔT) of daily temperature oscillation (Fig. 1) and the midpoint (T_{mid}) of the oscillation (Fig. 2) have little effect on uncertainty where $k_{\text{Oxygen}20^\circ}$ is $>20/\text{d}$.

Because of the relationship between travel time for propane and uncertainty in reaeration rate estimates, travel time is inversely related to uncertainty in estimates of P (Fig. 3). For relatively short travel times ($t_w < 0.5/k_{\text{Oxygen}20^\circ}$), uncertainty is similar for estimates of P and R, but for longer travel times, uncertainty is higher for estimates of R.

Absolute uncertainty (the gross magnitude of possible error) in estimates of P increases with photosynthetic rate but relative uncertainty de-

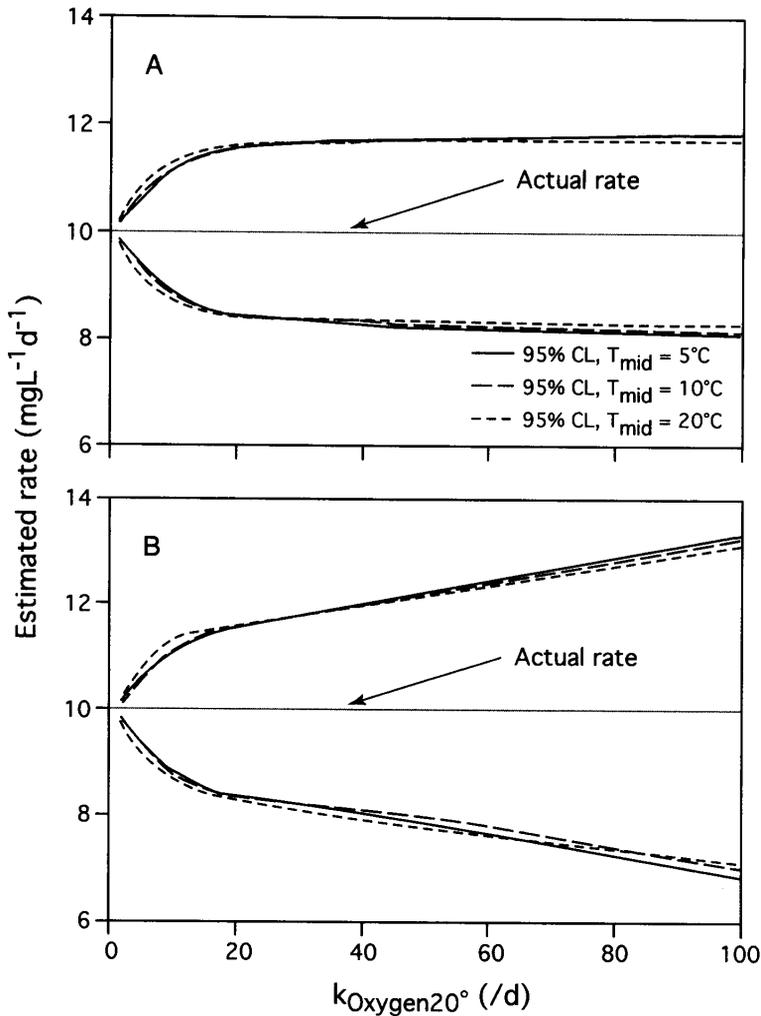


FIG. 2. Effects of midpoint temperature (T_{mid}) on 95% confidence limits (CL) for (A) photosynthesis and (B) respiration.

creases slightly (Fig. 4). At low reaeration rates, absolute uncertainty in R varies in a manner similar to uncertainty in P , but at higher $k_{Oxygen20^\circ}$, absolute uncertainty remains nearly constant, regardless of actual rate of R . As a result, relative uncertainty in estimates of R is considerably greater than relative uncertainty in estimates of P in streams with low metabolic rates.

Errors in the calibration of oxygen electrodes and in measurement of barometric pressure result in errors in measurements of stream oxygen concentration and the oxygen saturation deficit. These errors have almost no effect on uncertainty in estimates of P . Calibration errors, however, have a prominent effect on uncertainty in esti-

mates of R at high reaeration rates ($k_{Oxygen20^\circ} > 20/d$; Fig. 5).

Not surprisingly, the highest precision with the open-channel method is obtained in sluggish streams with high metabolic rates and the method may be inappropriate for very turbulent streams ($k_{Oxygen20^\circ} > 100/d$) with low rates of metabolism (Table 2). The open-channel method is suitable for moderately turbulent streams, however, if metabolic rates are moderately high or if estimates of P are the primary concern.

Reasonable CL (95% within 30% of the mean) for estimates of production can be achieved where P_d is at least $4.5 \text{ mg L}^{-1}\text{d}^{-1}$ and in less productive streams if $k_{Oxygen20^\circ}$ is $< 20/d$ (Fig. 6).

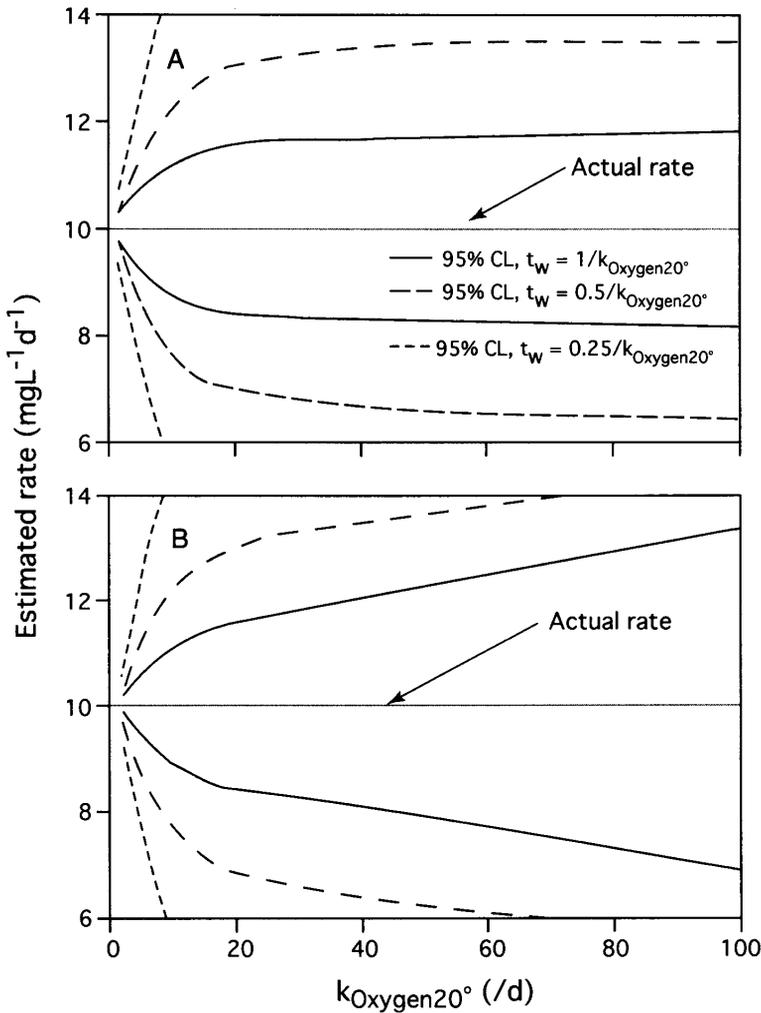


FIG. 3. Effects of travel time for propane (t_w) on 95% confidence limits (CL) for (A) photosynthesis and (B) respiration.

Similar CL for estimates of R are also possible, but only where metabolic rates are high relative to $k_{\text{Oxygen}20^\circ}$. At a $k_{\text{Oxygen}20^\circ}$ of 100/d, R_d must be roughly 3 times P_d for equivalent relative uncertainty in estimates of P and R .

Discussion

The open-channel method offers the possibility of system-level assessment of stream metabolism without the limitations of methods that hamper chamber approaches. Because open-channel estimates involve no true replication, the chief concern with this technique is uncer-

tainty. A Monte Carlo approach makes it possible to establish CL on metabolism estimates and to show where effort should be concentrated for improving confidence in these estimates.

Estimates of P and R behave differently with respect to uncertainty because R affects oxygen mass balance over the entire diel cycle but P only affects the rate of change of oxygen concentration during daylight hours. If $P_d = R_d$, uncertainty is similar for estimates of P and R in streams with high metabolic rates and low reaeration rates, but where $k_{\text{Oxygen}20^\circ}$ is high or metabolic rates are low, uncertainty is greater for estimates of R .

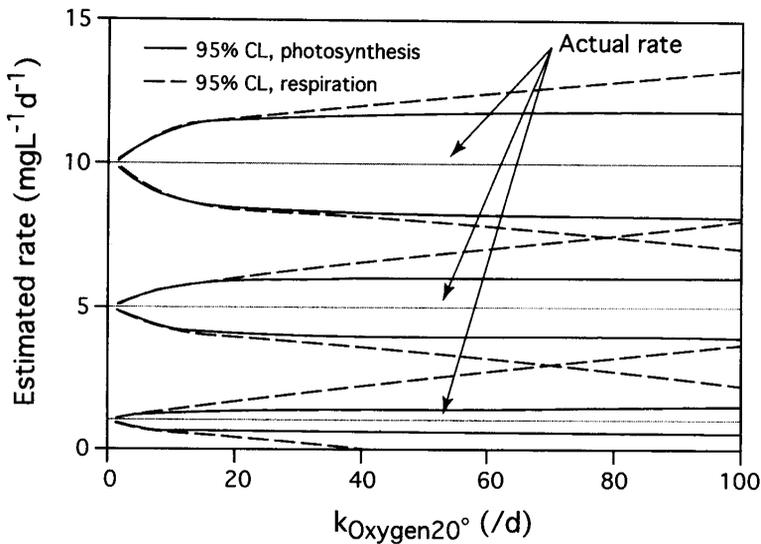


FIG. 4. Effects of actual rates of photosynthesis (P) and respiration (R) on 95% confidence limits (CL) for P and R.

Absolute uncertainty in estimates of R is strongly influenced by the magnitude of $k_{\text{Oxygen}20^\circ}$, uncertainty in $k_{\text{Oxygen}20^\circ}$, instrument calibration, and, at low reaeration rate, the actual rate of R. Increasing the travel time and taking multiple samples for propane analysis improve confidence in estimates of R. Further improvement in estimates of R results from more precise instrument calibration and measurement of barometric pressure in the field. Provided that a reasonable effort is made to meet these conditions (i.e., the SD for the mean of measured propane concentrations is $\sim 1.5\%$ of the actual value, the limit of detection for propane is 0.5 ppb, SD for oxygen electrode calibration is 0.01 mg/L, resolution of measurement for oxygen is 0.01 mg/L, and SD for measurement of barometric pressure is 0.6 mm Hg), respiration rates of $10 \text{ mg O}_2 \text{ L}^{-1} \text{ d}^{-1}$ can be estimated to within 35% of the actual rate in streams with reaeration rates for the oxygen slightly $>100/\text{d}$.

For estimates of P, uncertainty is relatively unaffected by the magnitude of reaeration if $k_{\text{Oxygen}20^\circ}$ is $>20/\text{d}$, but uncertainty is strongly affected by error in estimates of $k_{\text{Oxygen}20^\circ}$ and by the actual photosynthetic rate. Just as for estimates of R, estimates of P can be improved by precise estimates of reaeration rate, but instrument calibration and accuracy of barometric pressure readings have little effect on uncertainty for P. If uncertainty in estimates of $k_{\text{Oxygen}20^\circ}$

can be minimized through the use of long travel times, multiple samples for propane analysis, and sufficiently high upstream propane concentration, photosynthetic rates can be estimated to within 25% of the actual value in streams with reaeration rates well above $100/\text{d}$. Consequently, reliable open-channel estimates of P may be possible even in streams where P:R ratios or estimates of community R cannot be determined except through the use of chamber techniques.

The approach described here rests on the assumptions that there is no lateral inflow of water into the reach and there is no bubble formation during periods of high photosynthetic activity. If these assumptions are not met, uncertainty in metabolism estimates will be greater than predicted. The likelihood of lateral inflow increases with longer travel times, potentially negating the benefits associated with increasing travel time. Likewise, the higher relative precision of production estimates predicted for streams where P is high may disappear if bubbling occurs because oxygen lost from the stream as bubbles cannot be determined from changes in stream oxygen concentration and P may be underestimated. Although most stream reaches can receive lateral inflow at some time of the year and bubble formation can occur in slow-moving, productive streams, their contribution to error in estimates of stream metabolism has not been established. Therefore,

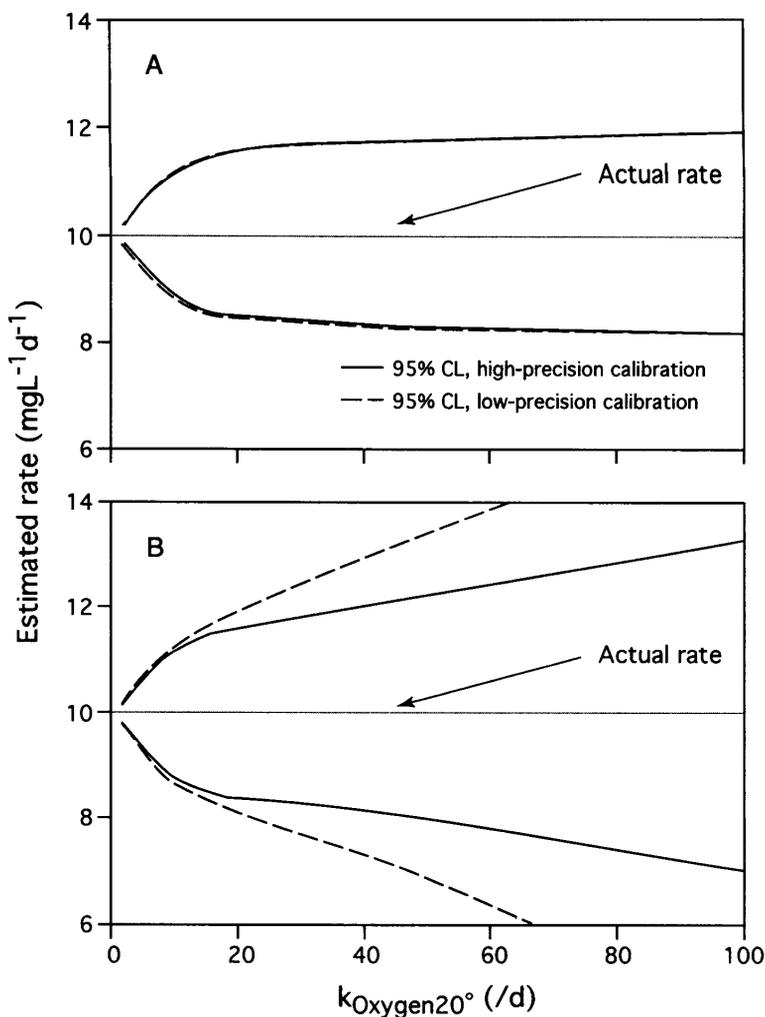


FIG. 5. Effects of calibration precision of the oxygen electrode on 95% confidence limits (CL) for (A) photosynthesis and (B) respiration. For the high-precision calibration, the standard deviation (SD) of the calibration is 0.010 mg O₂/L and the SD of measurement of barometric pressure is 0.6 mm Hg. For the low-precision calibration, the SD of the calibration is 0.025 mg O₂/L and the SD of measurement of barometric pressure is 2 mm Hg.

care must be taken to avoid situations in which lateral inflow or bubble formation could lead to large errors in metabolism estimates.

Although the precision and resolution of measurements used in simulations for this paper can be attained with good commercial sensors and may even be exceeded under some conditions (Yotsukura et al. 1983), this level of precision is probably rarely achieved in field measurements. Oxygen electrodes can be calibrated to within 0.02–0.03 mg/L, but only if special care is taken to maintain constant temperature

and full oxygen saturation during calibration (J. McCutchan, unpublished data). Estimates of pressure often are subject to considerable error when they are derived from elevation and are assumed to be constant over time, even though inexpensive (\$100–250) recording barometers are available. Although analytical precision for propane does not often directly limit precision of reaeration estimates, long travel times and high upstream propane concentrations can affect uncertainty. If the analytical SD for propane is 1.5% of the measured value, the necessary

TABLE 2. Sensitivity of the open-channel method in streams with high, intermediate, and low reaeration rates. 95% confidence limits (CL) of P_d (total daily photosynthesis) and R_d (daily respiration) are expressed as % of actual metabolic rates.

	$k_{\text{Oxygen}20^\circ}$ (/d)	95% CL (\pm % of actual rate)			
		Low metabolic rate ^a		High metabolic rate ^b	
		P_d	R_d	P_d	R_d
Steep stream	100	60	264	25	35
Intermediate stream	20	58	73	21	22
Sluggish stream	5	32	34	8	8

^a $P_d = R_d = 1 \text{ mg O}_2 \text{ L}^{-1} \text{ d}^{-1}$

^b $P_d = R_d = 10 \text{ mg O}_2 \text{ L}^{-1} \text{ d}^{-1}$

precision is obtained if travel time is at least $1/k_{\text{Oxygen}20^\circ}$ and the upstream propane concentration is at least 30 ppb. This relationship gives travel times of just over 2 h for $k_{\text{Oxygen}20^\circ} = 10/\text{d}$ and just under 15 min for $k_{\text{Oxygen}20^\circ} = 100/\text{d}$.

The flexibility of the Monte Carlo technique allows not only estimation of uncertainty for stream metabolism measurements, but also optimization of the open-channel method for individual reaches. With approximate values of T_{midr} , ΔT , $k_{\text{Oxygen}20^\circ}$, P , and R for a stream reach, it is possible to determine in advance the precision required for measurements of dissolved oxygen, temperature, barometric pressure, and $k_{\text{Oxygen}20^\circ}$ necessary to measure metabolic rates to a specified level of precision. Because the effects of im-

provements to measurements of individual variables on uncertainty in metabolism estimates can be explored, the Monte Carlo approach makes it possible to determine, for each location or set of conditions, the precision of open-channel metabolism estimates.

Acknowledgements

We thank Ron Hamilton and Laura Baumgartner who helped with the development of methods for instrument calibration and with field trials. We also thank D. M. Rosenberg, P. J. Mulholland, and 2 anonymous reviewers for their valuable comments during the preparation of this paper. This project was supported in part

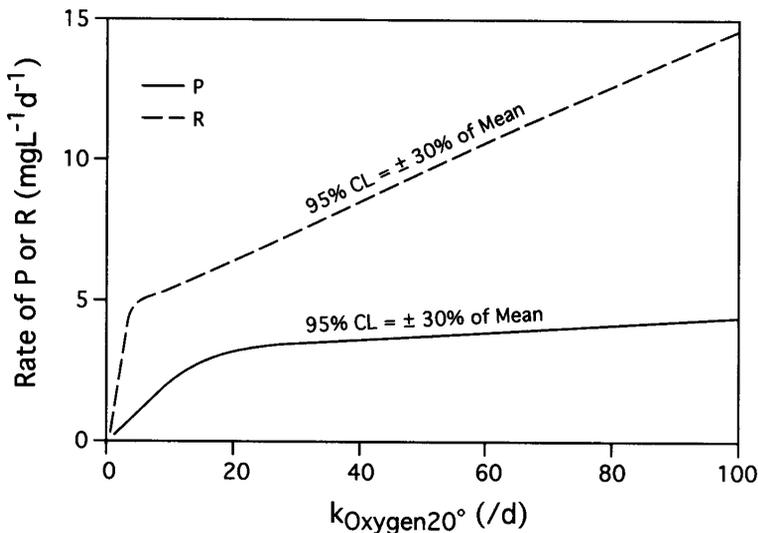


FIG. 6. Minimum metabolic rates necessary to obtain reasonable confidence limits (CL = $\pm 30\%$ of mean) for open-channel estimates of photosynthesis (P) and respiration (R).

by a grant from the National Science Foundation (DEB 9318205) and by the CIRES/CCHE Internship Program.

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Received: 31 July 1997

Accepted: 23 March 1998