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Assessment of random errors in multi-plot nitrous oxide flux gradient measurements

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A B S T R A C T

The multi-plot flux-gradient (FG) technique is well-suited for non-intrusive measurements of agricultural N_2O emissions for individually-treated field-scale plots across growing seasons at high temporal and spatial resolution. The degree of random error associated with N_2O flux measurements is unknown; knowledge of these errors will increase confidence in the flux measurements and strengthen comparisons of total N_2O emissions between treatments. An error estimation routine was developed to determine the random error (σ) associated with FG-measured fluxes (σ_F). The combination of a moving-block bootstrapping technique and the filtering method of Salesky et al. (2012) estimated the σ values for each variable used in calculating individual 30-min FG-derived fluxes. This error analysis was applied to a year-long dataset where a four-plot FG system measured N_2O fluxes semi-continuously in a soybean field in Southwestern Ontario, Canada, with each plot having different treatments affecting N_2O emissions. Errors of the concentration differences contributed the largest proportion to the σ_F values. The individual 30-min σ_F values did not correlate with the magnitude of the flux but were positively correlated with turbulence conditions. Random errors of N_2O fluxes greater than 45 ng N m^{-2} s^{-1} had values representative of 9% of the measured flux, whereas error of fluxes close to zero frequently exceeded the value of the measured flux. Cumulating the errors over the experiment reduced the degree of error associated with the cumulated total N_2O emissions with an average value of 31.5 g N ha^{-1}, which represented on average ± 5.5% of the total N_2O emissions. The proposed framework is applicable to other scalar fluxes being determined by the flux-gradient method.

1. Introduction

Micrometeorological measurements provide information on the exchange of greenhouse gases between agricultural land and the atmosphere (Nemitz et al., 2000; Denmead et al., 2008). Nitrous oxide (N_2O) is a potent greenhouse gas emitted by soils, thus measurements of N_2O fluxes are needed in order to test mitigation practices that reduce emissions (Reay et al., 2012; Snyder et al., 2014). Any measurement of N_2O emissions will have a degree of uncertainty. Knowledge of the uncertainty increases confidence in the flux measurements, and is necessary for comparisons between measurements (Richardson et al., 2012). Chamber methods are predominantly used for comparisons of N_2O emissions (Rochette et al., 2008; Venterea et al., 2011; Drewer et al., 2012; Xiaopeng et al., 2013; Burchill et al., 2014) as they are low-cost and require a small area for flux measurements, making it easier to implement replicated comparisons between several agricultural treatments. However, chamber measurements do not cover a large enough area to fully capture the spatial heterogeneity of N_2O emissions, and practical considerations have limited continuous measurements (Henault et al., 2012), particularly through the winter in cold climates. Eddy- covariance (EC) measurements provide long-term N_2O flux values that cover significant footprints (Molodovskaya et al., 2011; Jones et al., 2011), and methods have been developed to estimate the degree of uncertainty of EC measurements (Lenschow et al., 1994; Kroon et al., 2010; Mauder et al., 2013). EC measurements are not practical for plot comparisons as the frequency-response requirements necessitates multiple analyzers for multi-plot comparisons.

The multi-plot flux gradient (FG) approach provides an alternative to both chamber and EC methods to measure long-term fluxes for the purpose of treatment comparisons (Pattey et al., 2006; Wagner-Riddle et al., 2007; Phillips et al., 2007; Desjardins et al., 2010; Glenn et al., 2010; Maas et al., 2013; Laubach et al., 2016). This approach allows for semi-continuous, spatially integrated flux measurements for up to four different plots under similar soil and climatic conditions. Greater spatial coverage is achieved with FG measurements than chamber techniques, and long-term flux measurements can be obtained using one analyzer

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over large plots subjected to differing agricultural practices. The FG experimental design typically consists of one analyzer to sequentially measure concentration differences, one plot at a time, over time periods ranging from several months to several growing seasons. Information on the turbulent conditions is used in combination with the measured gradient to calculate the flux. Fluxes are cumulated over the measurement period to give total emissions and are then compared. Numerous studies have applied this methodology to examine the effects of management techniques on total emissions of the species of interest (Glenn et al., 2012; McMillan et al., 2014; Abalos et al., 2016) or the effects of management on the dynamics and drivers of trace gas fluxes (Furon et al., 2008; Kariyapperuma et al., 2012; Risk et al., 2014).

Similar to EC measurements, uncertainty quantification for FG measurements is challenging as treatment replication is typically limited. Uncertainty is therefore determined by evaluating several types of measurement errors. Measurement errors are generally classified as being either random or systematic. Systematic errors, also known as bias errors, shift the flux values in one direction or another, and can arise for FG measurements from inadequate instrument calibration, instrument offsets, undersampling of low frequency concentration signals (Lenschow et al., 1994), or inadequate parametrization of the FG equations (Loubet et al., 2013). Random errors reduce the precision of flux measurements and cannot be corrected for (Richardson et al., 2012). Sources of random errors are instrument noise (Blanc, 1983; Laubach and Kelliher, 2004; Mukherjee et al., 2014), heterogeneity in the flux footprint (Laville et al., 1997), and from the stochastic nature of turbulence (Mauder et al., 2013). Random error from the stochasticity of turbulence is of greater influence to the total uncertainty than sensor noise (Salesky and Chamecki, 2012; Mauder et al., 2013; Langford et al., 2015), and has not been evaluated for FG measurements.

The definition of random error given by Lumley and Panofsky (1964) is the variation of the sample mean, as measured by time-averaging using single-point instrumentation, from the true ensemble mean. This quantifies the degree of random error from the stochasticity of turbulence, and is the definition of random error used throughout this study. A consequence of measuring fluxes over finite time intervals in turbulent, variable conditions is the inability of flux measurements to converge to the true ensemble value (Lenschow et al., 1994; Mahrt, 1998; Laville et al., 1999; Salesky et al., 2012). The definition from Lumley and Panofsky (1964) is based on the principle that the error variance of an average from the ensemble mean (σ_f^2) approaches zero with increasing averaging time. Relating the properties of the variance with the autocorrelation function gives:

$$\sigma_f^2 = <\frac{1}{T}\int_0^T f\left(t'\right)dt' - \overline{f(t)}^2> = \frac{2<f'^2>}{T}\int_0^T \rho(t)dt \tag{1}$$

where $\langle f'^2 \rangle$ represents the ensemble variance, ρ is the autocorrelation function, and T the time period over which the measurements were taken. Integration of the autocorrelation function gives the integral time scale ($\mathfrak{I}$), such that the random error can be expressed as:

$$\sigma_f^2 \approx \frac{2\mathfrak{I}\langle f'^2 \rangle}{T} \tag{2}$$

In practice, $\langle f'^2 \rangle$ is replaced by the sample variance. Increased $\mathfrak{I}$ within the sampling interval is analogous to a decrease in the number of independent samples, thus increasing $\langle \sigma_f^2 \rangle$, which is akin to the impact of reducing the number of replicates in a standard replicated experimental design.

Several of the methods for estimating random error, expressed as the standard error $\sigma_f = (\sigma_f^2 n^{-1})^{0.5}$, where n is the number of independent samples, are based on the Lumley and Panofsky (1964) definition and thus rely on the value of the integral time scale (Lenschow et al., 1994; Mann and Lenschow, 1994; Finkelstein and Sims, 2001). Random error calculations for EC measurements typically use variations on Eq. (2) (Rannik et al., 2004; Peltola et al., 2014; Litt et al., 2015). The value of $\mathfrak{I}$ varies depending on the estimation technique, as $\mathfrak{I}$ can change with record length (Theunissen et al., 2008) and choices for the maximum lag time and the upper bound of the integration of ρ (Dias et al., 2004). Methods exist for σ_f estimations that are independent of $\mathfrak{I}$ to avoid this uncertainty. Bootstrapping methods have estimated random errors for turbulent quantities in flumes (Garcia et al., 2006; Theunissen et al., 2008; Amir et al., 2014) and in the atmospheric surface layer (Davies et al., 2003; Dias et al., 2004; Bernardes and Dias, 2010). Salesky and Chamecki (2012) estimated random errors of the turbulence statistics and stability parameters used in Monin–Obukhov similarity theory with the filtering method of Salesky et al. (2012) to avoid the use of integral scales. Bootstrapping or filtering methods are an intuitive alternative to Eq. (2); increased variability between means of either re-sampled or spatially-filtered sampled datasets indicates divergence from the ensemble mean. Salesky and Chamecki (2012) demonstrated the comparability between the filtering and bootstrapping methods and Eq. (2). These methods have not been applied to estimate σ_f of flux-gradient measurements.

The degree of non-convergence of the sample mean to the true ensemble mean has not been quantified for FG measurements. Guidelines and definitions for assessing random error of single-point EC measurements have been well-developed (Hollinger and Richardson, 2005; Billesbach, 2011; Richardson et al., 2012; Mauder et al., 2013). The quantification of random error for FG measurements differs from EC measurements in that the FG calculation requires measuring several different variables, all of which have differing degrees of random error. These individual σ_f values are then propagated through the FG calculation. Several studies have used error propagation to assess uncertainty of FG measurements, but with varying definitions of random error. Aspects related to random error, such as errors from limitations on instruments to resolve gradients (Laubach and Kelliher, 2004; Walker et al., 2006; McMillan et al., 2014), errors associated with instrument noise (Laville et al., 1997; Glenn et al., 2012; Mukherjee et al., 2014), or Monte Carlo simulations to assess the impact of the range of error on the uncertainty of the flux measurements (Mukherjee et al., 2014) all give information on various aspects of FG uncertainty. An assessment of the random error of all variables involved in FG flux calculations is needed to evaluate differences in N_2O emissions in multi-plot FG systems. Additionally, the contributions of each variable in the FG equation to the total random error of flux measurements is unknown.

This study quantified the degree of random error of individual 30-min flux measurements for a multi-plot FG experiment measuring fluxes of N_2O over the course of a year. A routine was developed to quantify the random error of the variables used to calculate FG fluxes using either the filtering method of Salesky and Chamecki (2012) or a bootstrapping algorithm. These methods used the high-frequency (10 or 20 Hz) data of each variable in the FG flux equation. Calculation of these errors allowed for (1) identification of the properties of random errors of the FG variables and their relationships with atmospheric conditions; (2) propagation of these errors through the FG equations to calculate the random error of the flux measurements; (3) characterization of the source of random error of the fluxes; and (4) evaluation of the random error effect on comparisons of N_2O emission from four plots by cumulating the random errors throughout the measurement period.

2. Methods

2.1. Field site

Data from one year of a multi-plot FG measurement campaign provided the information to analyze the random errors. Measurements of N_2O fluxes were conducted at the Elora Research Station (43°38′N 80° 25′W, 376 m elevation) in Elora, Ontario, Canada, from June 2009 to June 2011. The current study uses data from 2010. A companion paper (Congreves et al., 2016) presents the evaluation of the treatment