Atmospheric Environment 155 (2017) 189–198

Contents lists available at ScienceDirect

Atmospheric Environment

journal homepage: www.elsevier.com/locate/atmosenv

Designing efficient nitrous oxide sampling strategies in agroecosystems using simulation models

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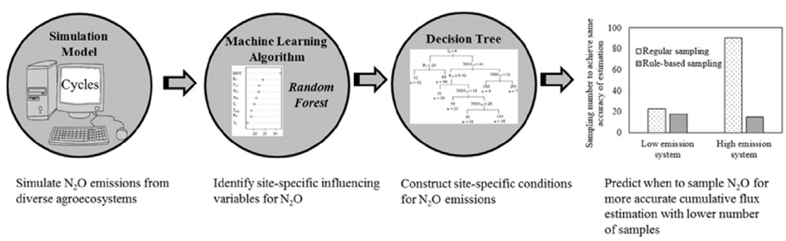
HIGHLIGHTS

- Nitrous oxide flux estimated from discrete measurements have unknown uncertainty.
- This uncertainty is location-specific for regular-interval sampling.
- Rule-based sampling yields better and less costly estimates than regular sampling.
- The performance of rule-based sampling is location and system specific.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 23 November 2016
Received in revised form 30 January 2017
Accepted 30 January 2017
Available online 31 January 2017

Keywords:
Cumulative nitrous oxide flux
Simulation model
Sampling
Fixed interval
Rule-based
Decision tree

ABSTRACT

Annual cumulative soil nitrous oxide (N_2O) emissions calculated from discrete chamber-based flux measurements have unknown uncertainty. We used outputs from simulations obtained with an agroecosystem model to design sampling strategies that yield accurate cumulative N_2O flux estimates with a known uncertainty level. Daily soil N_2O fluxes were simulated for Ames, IA (corn-soybean rotation), College Station, TX (corn-vetch rotation), Fort Collins, CO (irrigated corn), and Pullman, WA (winter wheat), representing diverse agro-ecoregions of the United States. Fertilization source, rate, and timing were site-specific. These simulated fluxes surrogated daily measurements in the analysis. We "sampled" the fluxes using a fixed interval (1–32 days) or a rule-based (decision tree-based) sampling method. Two types of decision trees were built: a high-input tree (HI) that included soil inorganic nitrogen (SIN) as a predictor variable, and a low-input tree (LI) that excluded SIN. Other predictor variables were identified with Random Forest. The decision trees were inverted to be used as rules for sampling a representative number of members from each terminal node. The uncertainty of the annual N_2O flux estimation increased along with the fixed interval length. A 4- and 8-day fixed sampling interval was required at College Station and Ames, respectively, to yield ±20% accuracy in the flux estimate; a 12-day interval rendered the same accuracy at Fort Collins and Pullman. Both the HI and the LI rule-based methods provided the same accuracy as that of fixed interval method with up to a 60% reduction in sampling events, particularly at locations with greater temporal flux variability. For instance, at Ames, the HI rule-based and the fixed interval methods required 16 and 91 sampling events, respectively, to achieve the same absolute bias of 0.2 kg N ha^{-1} yr^{-1} in estimating cumulative N_2O flux. These results suggest that

List of abbreviations: RF, Random Forest; DOY, day of year; T_{avg}, average air temperature; R, cumulative rainfall (and irrigation); I, net water inflow; SIN, total soil inorganic nitrogen; T, soil temperature; θ, volumetric soil water; HI, high input rule-based; LI, low input rule-based.

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http://dx.doi.org/10.1016/j.atmosenv.2017.01.052

using simulation models along with decision trees can reduce the cost and improve the accuracy of the estimations of cumulative N_2O fluxes using the discrete chamber-based method.

1. Introduction

Nitrous oxide (N_2O), a potent greenhouse gas (GHG), is mostly emitted from agricultural soils (IPCC Climate Change, 2007). This gas is produced through microbe-mediated processes, chiefly nitrification and denitrification (Firestone and Davidson, 1989). The temporal patterns of N_2O fluxes from agricultural soils are highly variable due to their episodic and transient nature, with marked diurnal and seasonal variations (Jacinthe and Dick, 1997; Smith et al., 2001; Flessa et al., 2002; Parkin, 2008). These emission events may occur in response to rainfall, irrigation, thawing, tillage, nitrogen (N) fertilization, and organic matter addition (Clayton et al., 1997; Oates et al., 2016; Reeves et al., 2016). Peak emission events can contribute about half of the growing season N_2O flux (Parkin and Kaspar, 2006). The high temporal variability makes the estimation of cumulative N_2O flux uncertain if measurements are not frequent or continuous (Parkin, 2008). However, assessing the impact of different management practices on N_2O emissions requires an accurate estimation of the cumulative flux.

In addition to the temporal variation, N_2O emissions vary spatially (Saha et al., 2016). Both time and space variations in N_2O fluxes are regulated by soil oxygen concentration (Smith and Dobbie, 2001), soil temperature (Parkin and Kaspar, 2006; Zhang et al., 2016), carbon (C) and mineral-N availability (Gillam et al., 2008), and microbial diversity (Regan et al., 2011). Weather conditions alter all these factors, causing a marked inter-year variability of N_2O fluxes from the same soil and management practices (Dobbie et al., 1999; Burchill et al., 2014). Since we have a limited ability to predict how these factors will drive N_2O emissions, sampling at representative times with time-discrete monitoring methods is challenging.

Soil N_2O flux is commonly measured by the non-steady state closed chamber method (Hutchinson and Mosier, 1981). This method is temporally discontinuous and usually applied on weekly to monthly fixed intervals (Dobbie and Smith, 2003). Low frequency sampling can miss a short-lived peak in-between sampling events, which will cause an underestimation of the cumulative flux. Thus, sampling at regular weekly or bi-weekly intervals does not ensure an accurate estimation of cumulative N_2O flux (Barton et al., 2015). It also adds samplings in periods with little N_2O emission. Furthermore, the same fixed interval sampling may produce a different uncertainty in cumulative flux estimates in different locations (Barton et al., 2015), or in the same location in different years, a variation that is as yet unknown. Automated chambers (Smith and Dobbie, 2001) and micrometeorological techniques (Wagner-Riddle and Thurtell, 1998) can provide high frequency measurements. However, these are expensive and have low spatial resolution which limits their use in plot-scale replicated studies or remote areas.

What is the best way to define an N_2O flux sampling strategy that minimizes uncertainty and cost in a given location? We propose to answer this question by a novel approach of using an agroecosystem simulation model as a tool to determine the error of different sampling strategies in estimating cumulative N_2O flux in a given location and set of management practices. Simulation models of agroecosystems typically operate on a daily or sub-daily time step, providing detailed outputs of the water and N balance components in the soil-plant system for many years. As long as the models satisfactorily represent the N_2O emission patterns and their drivers, the results can be conceived as surrogates of daily chamber-based flux measurements. The simulation outputs can be "sampled" with different strategies and determine which ones render the lowest uncertainty and cost at a given location and management system.

We further propose to apply statistical methods such as Classification and Regression Trees (CART, Breiman et al., 1984) and Random Forests (RF) (Breiman, 2001; Liaw and Wiener, 2002) to the daily simulation output to cluster the daily N_2O fluxes into groups that can be identified by specific properties (for example, precipitation, evapotranspiration or N fertilization rate in prior days). These properties can become rules for sampling, leading to a decision support tool for field N_2O monitoring. This strategy is hereafter referred to as rule-based sampling.

Our goal is to combine the output of simulation models with statistical methods to design a robust strategy for N_2O sampling that is less expensive than regular fixed interval sampling. The research questions are: 1) How do different fixed interval sampling frequencies affect the uncertainty in estimating cumulative N_2O flux? 2) Does the relative error of a given sampling frequency vary across soil, climate, and management scenarios? 3) Is it possible to use simulation models to build decision tree based N_2O sampling strategies that are cost effective? To answer these questions, we simulated and analyzed N_2O emissions in four sites in the United States (US) with diverse soil, climate, management practices, and temporally distinct N_2O emission patterns.

2. Materials and methods

2.1. Cycles model description

Cycles is a process-based, multi-year, multi-crop, and multi-soil layer simulation model that runs at a daily time step, with hydrology simulated with an adaptive sub-daily time step. It produces daily outputs of N_2O flux along with other biogeochemical fluxes. Cycles has modules to represent plant growth based on radiation and transpiration use efficiency (Stöckle et al., 2008), coupled soil C and N cycling (White et al., 2014), soil water infiltration and redistribution, and the effect of management practices on biogeochemical processes. Cycles can simulate monoculture rotations, polycultures, and relay crops. The inputs required to run Cycles are: i) latitude, elevation, and daily weather data, ii) layer-by-layer initial soil profile properties (layer thickness, texture, bulk density, hydraulic properties, organic matter), iii) crop sequence, and iv) management operations (fertilization, irrigation, residue addition, tillage, harvest). Earlier tests of CropSyst (Stöckle et al., 2003) and C-Farm (Kemanian and Stöckle, 2010) are applicable to Cycles as they share several modules; however, the N_2O emission algorithm in Cycles has been modified recently to accommodate N_2O emissions from nitrification.

Cycles simulates N_2O flux from nitrification and denitrification. For each soil layer, the amount of N_2O derived from nitrification depends on the amount of ammonium nitrified and the air filled porosity, which is calculated from soil porosity and volumetric water content. The N_2O derived from denitrification depends on the