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From Lab to Field: Streamlined CRDS-Based N_2O Isotope Analysis for Source Identification in Agricultural Soils

JULIUS C. HAVSTEEN[1], MEHR FATIMA[2], SIMONE BRUNAMONTI[1], ANDREA POGÁNY[3], THOMAS HAUSMANINGER[2], BENJAMIN WOLF[4], REINHARD WELL[5] AND JOACHIM MOHN[6]

[1]Empa, Laboratory for Air Pollution / Environmental Technology
[2]VTT Technical Research Center of Finland Ltd
[3]Physikalisch-Technische Bundesanstalt
[4]Karlsruhe Institute of Technology (KIT), Institute of Meteorology and Climate Research, Atmospheric Environmental Research (IMK-IFU)
[5]Thünen Institute of Climate-Smart Agriculture
[6]Empa

Nitrous oxide (N_2O) is a potent greenhouse gas with a global warming potential about 300 times that of CO_2. Its rising atmospheric concentrations and critical role in climate change necessitates a deep understanding of its production and consumption pathways. Agricultural soils are the major anthropogenic source for N_2O emissions, and therefore research into the responsible biogeochemical processes, such as nitrification and denitrification, is essential for effectively assessing mitigation strategies.

Recent advances in cavity ring-down spectroscopy (CRDS) have enabled high-precision measurement of N_2O isotopic species at ambient concentrations. CRDS analysis surpasses traditional isotope ratio mass spectrometry (IRMS) with respect to its site selectivity for ^{15}N substitution and on-site capability. However, the inherent complexity of spectral fitting in CRDS measurements that arises from fundamental physical parameters such as gas matrix-dependent pressure broadening and spectral interferences as well as instrumental drift and non-linearity necessitates extensive post-processing to extract reliable data.

This work presents a comprehensive correction and calibration protocol for laser spectrometers, exemplified by N_2O isotopic data ($\delta^{15}N^{\alpha}$, $\delta\ ^{15}N^{\beta}$, $\delta^{18}O$) obtained from a Picarro G5131-*i* isotopic and gas concentration analyser. While the focus application in our current work is the analysis of N_2O emitted from agricultural soils using a specific analyser model, the general MATLAB code underpinning our approach is adaptable to a wide range of gas species, i.e. analyser models or brands. Specifically, the protocol establishes the theoretical and mathematical framework required for the corrections, outlines a logical sequence for their application, and includes an error propagation analysis to quantify associated uncertainties.

Applied to N_2O isotope data from an automated setup for autonomous analysis of up to 32 bag samples collected on a weekly base from automated flux chambers on agricultural soils, our protocol significantly reduces post-processing time and enhances the data quality. We will show exemplary data for a fertilizer study, which indicates differing shares of N_2O derived from nitrification and denitrification, providing important parameters to improve soil biogeochemical models. More generally, we aim to enable researchers to obtain high-quality isotope data from CRDS and similar instruments, ultimately contributing to standardized community guidelines for data post-processing.