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goFlux: A user-friendly way to calculate GHG fluxes yourself, regardless of user experience

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Software

- Review
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Summary

This new R package `goFlux` has been developed for calculating greenhouse gas (GHG) flux estimates from static chamber measurements. Compared to previous software developed for the same purpose, the `goFlux` package is not limited to the linear regression approach (LM), but also estimates GHG fluxes from a non-linear regression approach, the Hutchinson and Mosier model (HM). An automatic selection procedure has been implemented in the package to help users select the best flux estimate (LM or HM) based on objective criteria. In addition, this package can be used to import raw data directly downloaded from a vast selection of instruments (LI-COR, LGR, GAIA2TECH, Gasmet, Picarro and PP-Systems).

The package is divided into five steps: 1. import raw data into R; 2. identify measurements; 3. calculate GHG flux estimates (LM and HM); 4. automatically select the best flux estimate (LM or HM) based on our default choices of objective criteria; 5. and visually inspect the results on plots that can be saved as pdf. For a detailed protocol on how to use this package, visit the webpage https://qepanna.quarto.pub/goflux/.

Statement of need

Non-steady state chambers are widely used for measuring soil greenhouse gas (GHG) fluxes, such as CO_2, CH_4, N_2O, NH_3, CO, and water vapor (H_2O). While linear regression (LM) is commonly used to estimate GHG fluxes, this method tends to underestimate the pre-deployment flux (f_0). Indeed, non-linearity is expected when the gas concentration increases or decreases inside a closed chamber, due to changes in gas gradients between the soil and the air inside the chamber. In addition, lateral gas flow and leakage contribute to non-linearity. Many alternative to LM have been developed to try and provide a more accurate estimation of f_0, for instance the method of Hutchinson & Mosier (1981) (HM), which was implemented in the `HMR` package by Pedersen et al. (2010). However, non-linear models have a tendency to largely overestimate some flux measurements, due to an exaggerated curvature. Therefore, the user is expected to decide which method is more appropriate for each flux estimate. With the advent of portable greenhouse gas analyzers (e.g. Los Gatos Research (ABB) laser gas analyzers), soil GHG fluxes have become much easier to measure, and more efficient ways to calculate these flux estimates are needed in order to process large amounts of data. A recent approach was developed by Hüppi et al. (2018) to restrict the curvature in the HM model for a more reliable flux estimate. In the HM model, the curvature is controlled by the kappa parameter. Hüppi et al. (2018) suggest the use of the kappa.max to limit the maximal curvature allowed in the model (see their R package `gasfluxes`, available on the CRAN). This procedure introduces less arbitrary decisions in the flux estimation process.

Previous software developed to calculate GHG fluxes are limited in many aspects that the `goFlux` package is meant to overcome. Most are limited to the linear regression approach (e.g. Flux Puppy, and the R packages `flux` (Jurasinski et al., 2022) and `FluxCalR` (Zhao, 2019)), others do not include data pre-processing (e.g. the R packages `HMR` (Pedersen et al., 2010), `flux` and `gasfluxes` (Fuss, 2023)), or if they do, they are compatible with only a few designated systems (e.g. Flux Puppy and `FluxCalR`), and almost none include an automatic selection of the best flux estimate (LM or HM) based on objective criteria.

This new R package, `goFlux` is meant to be "student proof", meaning that no extensive knowledge or experience is needed to import raw data into R, choose the best model to calculate fluxes (LM or HM), quality check the results objectively and obtain high quality flux estimates. The package contains a wide range of functions that allows the user to import raw data from a variety of instruments (LI-COR, LGR, GAIA2TECH, Gasmet, Picarro and PP-Systems); calculate fluxes from a variety of GHG (CO_2, CH_4, N_2O, NH_3, CO and H_2O) with both linear (LM) and non-linear (HM) flux calculation methods; interactively identify measurements (start and end time) if there are no automatic chamber recordings (e.g. LI-COR smart chamber); plot measurements for easy visual inspection; and quality check the measurements based on objective criteria.

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