ConFluxPro: A toolkit for soil gas analysis

Valentin Gartiser[1,2]**, Verena Lang**[1]**, and Martin Maier**[2]

1 Forest Research Institute, Freiburg, Germany **2** Soil Physics, Department of Crop Sciences, Göttingen, Germany

Summary

`ConFluxPro` is an R-package to model soil gas fluxes with the flux-gradient method (FGM). The FGM is a cost-effective way to measure fluxes and production rates of gases in soils (Maier & Schack-Kirchner, 2014). It relies on the principle that gas exchange in soils is driven by molecular diffusion and can therefore be described by Fick's first law of diffusion. In situ, it requires measuring vertical concentration profiles of soil gases and parameters to estimate the diffusivity of the soil. Flux rates can then be modeled by deriving concentration gradients and diffusion coefficients of soil gases.

We developed `ConFluxPro` to assist along the entire modeling process, from data handling and preparation to flux modeling and beyond. The package (I) provides object classes for the preparation, combination and modification of soil gas and physical data, (II) implements different common FGM models, (III) introduces an inverse modeling approach, (IV) provides functions for post-hoc calibration and (V) uncertainty estimation of the model results. All this functionality was built to be modular and user-friendly on the outside with robust internals handling more complex data manipulations. This makes it easy to implement an individual approach to the FGM, while improving the reproducibility of the analysis.

Statement of need

The FGM is conceptually simple and has been applied in numerous studies. However, codes or evaluation files have often not been shared publicly and there are differences between individual implementations. For example, concentration gradients may be calculated using a linear regression (Tang et al., 2003), simple differences between depths (De Jong & Schappert, 1972) or by fitting exponential functions (Davidson et al., 2006). While there may be valid reasons to favour one approach over another within any study, this makes it hard to compare results between studies. Furthermore, the uncertainty of the approach due to soil heterogeneity and measurement uncertainty is often not considered. Still, the FGM is uniquely equipped to address questions on subsurface processes and for long-term measurement (Maier et al., 2020). The goal of `ConFluxPro` was to make the FGM easy to implement, flexible and reproducible.

A first challenge in applying the FGM is to combine the various input parameters needed for the flux calculation. These may be from different sources (online measurement or soil samples), be of different types (volumetric or point measurements) and have different spatial and temporal resolutions. For this reason, `ConFluxPro` first implements different functions and object classes to shape the data into a predictable frame. Once the data is unified in this way, all subsequent operations can be mostly handled internally. This

limits the need for user intervention, both making it easier to implement and reducing an important source of error in the analysis.

Apart from the commonly used approaches, `ConFluxPro` also comes with an inverse model to estimate profiles of gas production rates similar to Schack-Kirchner et al. (2011). Instead of deriving concentration gradients from the measurements, the model calculates a concentration profile form assumed production (or consumption) rates. This profile is then fit to the measurements by algorithmically optimizing the production rates. The advantage of the inverse model is that the entire profile is consistently described by functions derived from physical laws. While this approach is conceptually more advanced, it is as easy to use within the package.

Soil heterogeneity and measurement error introduces uncertainty in FGM models. This is addressed in `ConFluxPro` in two ways. First, we implemented a calibration approach to reduce the differences between modeled and reference flux rates (e.g. from chamber measurements). Second, a bootstrapping approach gives an estimate of the model uncertainty introduced from the variability of the input parameters.

`ConFluxPro` is a versatile toolkit to model soil gas fluxes with the FGM. During development, we have already used it in multiple studies (Jochheim et al., 2022; Maier et al., 2020). The scientific background of the methods is described in Gartiser et al. (2025). By sharing this package we hope to make it easier to implement the FGM in future studies, furthering our knowledge of important soil processes.

Related software

To our knowledge, there is currently no other comprehensive implementation of the FGM. An approach in `Python` is described in Bittelli et al. (2015). The package `neonSoilFlux` (Zobitz & Ayres, 2024) implements the FGM specificly to the National Ecological Observatory Network (NEON). There are multiple R-packages to help with the analysis of chamber measurement data, `gasfluxes` (Fuss, 2016), `goFlux` (Rheault et al., 2024) and `FluxCalR` (Zhao, 2019).

Funding

References

Bittelli, M., Campbell, G. S., & Tomei, F. (2015). *Soil physics with Python*. Oxford University Press. https://doi.org/10.1093/acprof:oso/9780199683093.001.0001

Davidson, E. A., Savage, K. E., Trumbore, S. E., & Borken, W. (2006). Vertical partitioning of CO_2 production within a temperate forest soil. *Global Change Biology*, *12*(6), 944–956. https://doi.org/10.1111/j.1365-2486.2005.01142.x

De Jong, E., & Schappert, H. J. V. (1972). Calculation of soil respiration and activity from CO_2 profiles in the soil. *Soil Science*, *113*(5), 328–333. https://doi.org/10.1097/00010694-197205000-00006

Fuss, R. (2016). Gasfluxes: Greenhouse gas flux calculation from chamber measurements. In *CRAN: Contributed Packages*. The R Foundation. https://doi.org/10.32614/cran.package.gasfluxes

Gartiser, V., Lang, V., & Maier, M. (2025). A new approach to address soil heterogeneity as a source of uncertainty in the Flux-Gradient Method: CO_2 case studies. *European Journal of Soil Science*, *76*(3). https://doi.org/10.1111/ejss.70126

Jochheim, H., Wirth, S., Gartiser, V., Paulus, S., Haas, C., Gerke, H. H., & Maier, M. (2022). Dynamics of soil CO_2 efflux and vertical CO_2 production in a European Beech and a Scots Pine forest. *Frontiers in Forests and Global Change*, *5*. https://doi.org/10.3389/ffgc.2022.826298

Maier, M., Gartiser, V., Schengel, A., & Lang, V. (2020). Long term soil gas monitoring as tool to understand soil processes. *Applied Sciences*, *10*(23), 8653. https://doi.org/10.3390/app10238653

Maier, M., & Schack-Kirchner, H. (2014). Using the Gradient Method to determine soil gas flux: A review. *Agricultural and Forest Meteorology*, *192–193*, 78–95. https://doi.org/10.1016/j.agrformet.2014.03.006

Rheault, K., Christiansen, J. R., & Larsen, K. S. (2024). goFlux: A user-friendly way to calculate GHG fluxes yourself, regardless of user experience. *Journal of Open Source Software*, *9*(96), 6393. https://doi.org/10.21105/joss.06393

Schack-Kirchner, H., Kublin, E., & Hildebrand, E. E. (2011). Finite-element regression to estimate production profiles of greenhouse gases in soils. *Vadose Zone Journal*, *10*(1), 169–183. https://doi.org/10.2136/vzj2009.0193

Tang, J., Baldocchi, D. D., Qi, Y., & Xu, L. (2003). Assessing soil CO_2 efflux using continuous measurements of CO_2 profiles in soils with small solid-state sensors. *Agricultural and Forest Meteorology*, *118*(3–4), 207–220. https://doi.org/10.1016/s0168-1923(03)00112-6

Zhao, J. (2019). FluxCalR: A R package for calculating CO_2 and CO_4 fluxes from static chambers. *Journal of Open Source Software*, *4*(43), 1751. https://doi.org/10.21105/joss.01751

Zobitz, J., & Ayres, E. (2024). neonSoilFlux: Compute soil carbon fluxes for the National Ecological Observatory Network sites. In *CRAN: Contributed Packages*. The R Foundation. https://doi.org/10.32614/cran.package.neonsoilflux