

# **A direct comparison between field-measured and sensor-based estimates of soil carbon dioxide flux across six National Ecological Observatory Network sites enabled by the `neonSoilFlux` R package**

## **1 Introduction**

Soils contain the largest reservoir of terrestrial carbon (Jobbágy & Jackson, 2000). A critical component of this reservoir is soil organic matter, the accumulation of which is influenced by biotic factors such as above-ground plant inputs (Jackson et al., 2017). These inputs in turn are influenced by environmental factors such as growing season length, temperature, and moisture (Desai et al., 2022), which also affect the breakdown of soil organic matter and its return to the atmosphere. Across heterogeneous terrestrial landscapes, the interplay between these biotic and abiotic factors influence the size of the soil contribution to the terrestrial carbon sink (Friedlingstein et al., 2023). However, the heterogeneity of these processes across diverse ecosystems in the context of rapid environmental change leads to large uncertainty in the magnitude of this sink in the future, and thus a pressing need to quantify changes in soil carbon pools and fluxes across scales.

Ecological observation networks such as the United States' National Ecological Observatory Network (NEON) and others (e.g. FLUXNET or the Integrated Carbon Observation System) present a significant advancement in the nearly continuous observation of biogeochemical processes at the continental scale. Notably, at 47 core terrestrial sites across the continental United States, NEON provides half-hourly measurements of soil CO<sub>2</sub> concentration, temperature, and moisture at different vertical depths. Each of these NEON sites also encompasses measurements of the cumulative sum of all ecosystem carbon fluxes in an airshed using the eddy covariance technique (Baldocchi, 2014). Soil observations provided by NEON are on the same timescale and standardized with eddy covariance measurements from FLUXNET. These

types of data (NEON and FLUXNET) can be used to reconcile differences between model-derived or data-estimated components of ecosystem carbon flux (Jian et al., 2022; Luo et al., 2011; Phillips et al., 2017; J. Shao et al., 2015; P. Shao et al., 2013; Sihi et al., 2016).

Beyond direct observations of soil CO<sub>2</sub> concentrations and other environmental variables such as moisture or temperature, estimated or observed soil carbon fluxes are a key metric for understanding change in soil carbon pools over time (Bond-Lamberty et al., 2024). A soil carbon flux to the atmosphere ( $F_S$ , units  $\mu\text{mol m}^{-2} \text{s}^{-1}$ ), represents the aggregate process of transfer of soil CO<sub>2</sub> to the atmosphere from physical and biological processes (e.g. diffusion and respiration). Measurements of soil carbon fluxes can be coupled with empirical or process models of soil carbon. Soil carbon fluxes can be assumed to encompass soil carbon respiration from autotrophic or heterotrophic sources (Davidson et al., 2006), typically assumed to be static across the soil biome and modeled with a exponential  $Q_{10}$  paradigm (Bond-Lamberty et al., 2004; Chen & Tian, 2005; Hamdi et al., 2013).

One method by which  $F_S$  is measured in the field is through the use of soil chambers in a closed, well-mixed system (Norman et al., 1997) with headspace trace gas concentrations measured with an infrared gas analyzer (IRGA).  $F_S$  can also be estimated from soil CO<sub>2</sub> measurements at different depths in the soil using the flux-gradient method. This method is an approach that uses conservation of mass to calculate flux at a vertical soil depth  $z$  at steady state by applying Fick’s law of diffusion. A simplifying assumption for the flux-gradient method is that there no mass transfer in the other spatial dimensions  $x$  and  $y$  (Maier & Schack-Kirchner, 2014). The diffusivity profile, a key component of this calculation, varies across the soil depth as a function of soil temperature, soil volumetric water content, atmospheric air pressure, and soil bulk density (Millington & Shearer, 1971; Moldrup et al., 1999).

Databases such as the Soil Respiration Database (SRDB) or the Continuous Soil Respiration Database (COSORE) add to the growing network of resources for making collected observations of soil fluxes available to other workers (Bond-Lamberty, 2018; Bond-Lamberty et al., 2020; Bond-Lamberty & Thomson, 2010; Jian et al., 2021; Jiang et al., 2024). However, these databases currently encompass primarily direct soil measurements of fluxes (i.e. those using methods like the closed-chamber method described above). Currently, NEON provides all measurements to calculate  $F_S$  from Fick’s law, but soil flux as a derived data product was descope from the initial network launch due to budget constraints (Berenbaum et al., 2015). Deriving estimates of  $F_S$  using continuous sensor data across NEON sites thus represents a high priority.

This study describes an R software package, `neonSoilFlux`, that can be used to derive a standardized estimate of  $F_S$  at all terrestrial NEON sites. After calculating these flux estimates, we then validated them against direct chamber-based field observations of soil carbon dioxide flux from a subset of terrestrial NEON sites spanning six states.

Key objectives of this study are to:

1. Apply the flux-gradient method estimate soil CO<sub>2</sub> flux from continuous sensor measurements across NEON sites.
2. Benchmark estimated soil carbon fluxes against field measurements (e.g. data from SRDB/COSORE, direct measurements of soil flux).
3. Identify sources of error in the flux-gradient approach across diverse sites in order to guide future work.

## 2 Materials and Methods

### 2.1 Field methods

#### 2.1.1 Focal NEON Sites

In order to acquire field data to validate model predictions of flux, we selected six terrestrial NEON sites for analysis. We conducted field measurement campaigns at these sites, which span a range of environmental gradients and terrestrial domains (Table 1). SJER, SRER, and WREF were visited during May and June of 2022, and WOOD, KONZ, and UNDE during May and June of 2024.

Over the course of two field campaigns in 2022 and 2024, we conducted week-long visits at each site. In consultation with NEON field staff, we first selected a specific plot in the soil sampling array to maximize the concurrent availability of sensor data. We then made measurements of flux on an hourly or half-hourly interval for 8 hours each day after letting temporarily-installed soil collar(s) equilibrate for approximately 24 hours.

Table 1: Listing of NEON sites studied for field work and analysis.  $\overline{T_S}$ : average soil temperature during field measurements.  $\overline{SWC}$ : average soil water content during field measurements

Site (NEON site ID)	Location	Ecosystem type	Mean annual temperature	$\overline{T_S}$ (°)	Mean annual precipitation	$\overline{SWC}$ (%)
Santa Rita Experimental Range (SRER)	31.91068, -110.83549	Shrubland	19.3°C	47.6°	346 mm	4.0%
San Joaquin Experimental Range (SJER)	37.10878, -119.73228	Oak woodland	16.4°C	41.7°	540 mm	1.2%
Wind River Experimental Forest (WREF)	45.82049, -121.95191	Evergreen forest	9.2°C	15.3°	2225 mm	27.2%
Chase Lake National Wildlife Refuge (WOOD)	47.1282, -99.241334	Restored prairie grassland	4.9°C	14.9°	495 mm	14.9%

Table 1: Listing of NEON sites studied for field work and analysis.  $\overline{T_S}$ : average soil temperature during field measurements.  $\overline{SWC}$ : average soil water content during field measurements

Site (NEON site ID)	Location	Ecosystem type	Mean annual temperature	$\overline{T_S}$ (°)	Mean annual precipitation	$\overline{SWC}$ (%)
Konza Prairie Biological Station (KONZ)	39.100774, -96.563075	Tallgrass Prairie	12.4°C	23.4°	870 mm	23.4%
University of Notre Dame Environmental Research Center (UNDE)	46.23391, -89.537254	Deciduous forest	4.3°	13.0°	802 mm	13.0%

### 2.1.2 Soil collar placement

Either one (2022 sampling campaign) or two (2024 sampling campaign) PVC soil collars (FIXME: diameter) were installed in close proximity to the permanent NEON soil sensors at each site. The soil plot where measurements was taken was chosen at each site in consultation with NEON staff to maximize likelihood of quality soil sensor measurements during the duration of the IRGA measurements at each site.

IN PROGRESS: Add graphic of soil plot layout and placement of soil collar(s) – could make diagram in OmniGraffle?

### 2.1.3 Infrared gas analyzer measurements of soil CO<sub>2</sub> flux

During the summer 2022 field campaign, a LI-COR 6800 with soil flux chamber attachment was used to measure soil fluxes for 8 hours each day on an hourly interval. During the summer 2024 field campaign, the LI-6800 measurements were taken on a half-hourly interval and were paired with an automated soil flux chamber setup (FIXME multiplexer, IRGA, chamber model numbers) that made automated measurements on a half-hourly interval 24 hours a day while we were on site. Each instrument was paired with a soil temperature and moisture probe (FIXME: Stevens model #) that was used to make soil temperature and moisture measurements concurrent with the CO<sub>2</sub> flux measurements.

IN PROGRESS: Dead bands, measurement duration, instrument self-testing.

### 2.1.4 Post-collection processing of data

IN PROGRESS: LI-COR SoilFluxPro software to assess dead band and measurement duration.

## 2.2 neonSoilFlux R package

We developed an R package (`neonSoilFlux`; <https://CRAN.R-project.org/package=neonSoilFlux>) to compute half-hourly soil carbon fluxes and uncertainties from NEON data. The objective of the `neonSoilFlux` package is a unified workflow soil data acquisition and analysis that supplements existing data acquisition software through the `neonUtilities` R package (<https://CRAN.R-project.org/package=neonUtilities>). Figure 1 outlines the basic workflow of the package.

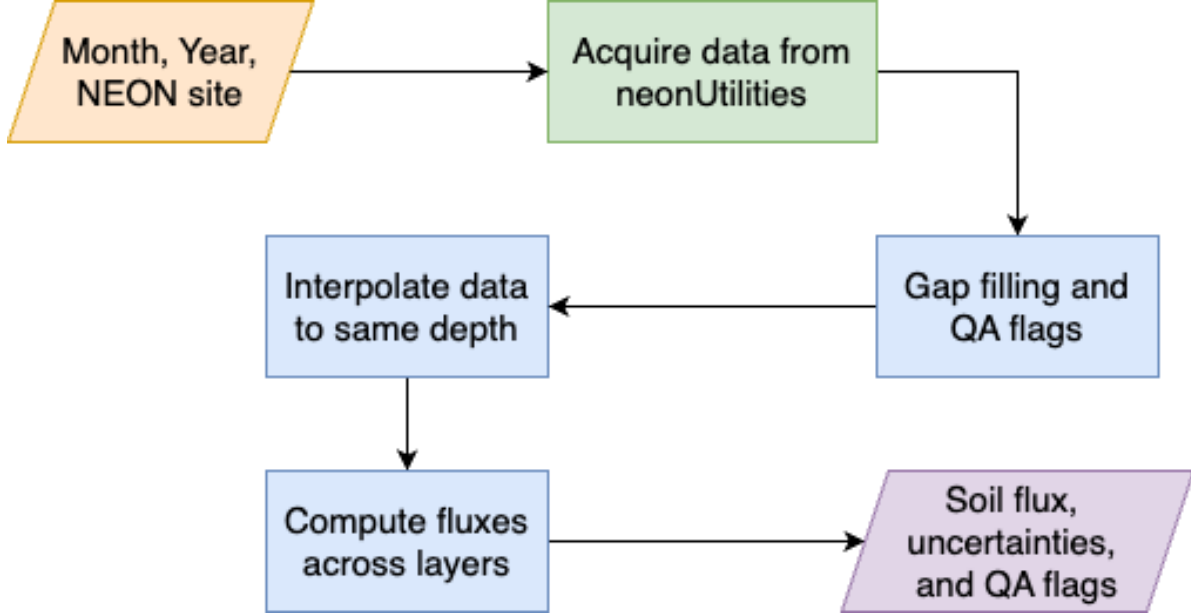


Figure 1: Diagram of `neonSoilFlux` R package. For a given month and NEON site, the package acquires all relevant data to compute  $F_S$  using the `neonUtilities` R package. Data are gap-filled according to reported QA flags and interpolated to the same measurement depth before computing the soil flux, uncertainties, and final QA flags.

At a given NEON observation there are five different replicate soil sensor arrays, with each sampling at five different soil depths (Figure 2). The `neonSoilFlux` package acquires measured soil water content (National Ecological Observatory Network (NEON), 2024e), soil  $\text{CO}_2$  concentration (National Ecological Observatory Network (NEON), 2024b), barometric pressure (National Ecological Observatory Network (NEON), 2024a), soil temperature (National Ecological Observatory Network (NEON), 2024d), and soil properties (e.g. bulk density) (National Ecological Observatory Network (NEON), 2024c). The static soil properties are periodically collected and assumed to be constant for the monthly observation period.

The workflow to computing a value of  $F_S$  with the `neonSoilFlux` consists of three primary steps. First, NEON data are acquired for a given site and month via the `neonUtilities` R package (yellow parallelogram and green rectangle in Figure 1 and Panel a in Figure 2).

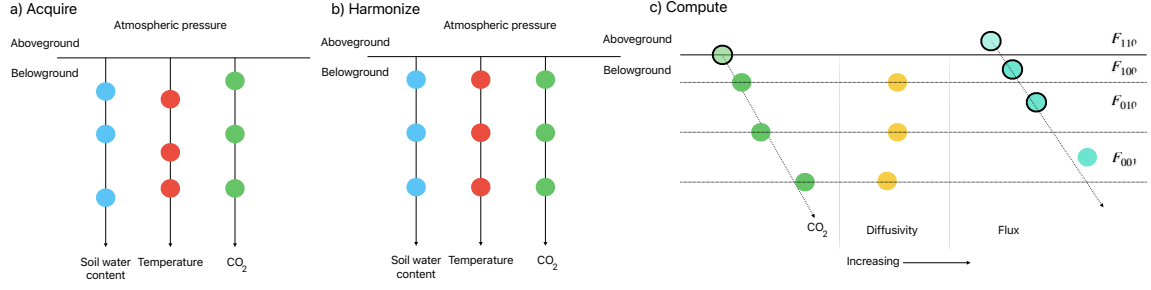


Figure 2: Model diagram for data workflow for the `neonSoilFlux` R package. a) Acquire: Data are obtained from given NEON location and horizontal sensor location, which includes soil water content, soil temperature, CO<sub>2</sub> concentration, and atmospheric pressure. All data are screened for quality assurance, with gap-filling of missing data reported. b) Any belowground data are then harmonized to the same depth as CO<sub>2</sub> concentrations using linear regression. c) The flux across a given depth is computed via Fick's law, denoted with  $F_{ijk}$ , where  $i, j$ , or  $k$  are either 0 or 1 denoting the layers the flux is computed across ( $i$  = closest to surface,  $k$  = deepest).  $F_{000}$  represents a flux estimate where the gradient  $dC/dz$  is the slope of a linear regression of CO<sub>2</sub> with depth.

Acquired environmental data can be exported to a comma separated value file for additional analysis. Quality assurance (QA) flags with an observation are reported as an indicator variable.

The next step is harmonizing the data to compute soil fluxes across soil layers. This step consists of three different actions (blue rectangles in Figure 1 and Panel b in Figure 2). If a given observation did is reported as not passing a quality assurance check we applied a gap filling method to replace that measurement with its monthly mean at that same depth (Section 2.2.1). Belowground measurements of soil water and soil temperature are then interpolated to the same depth as soil CO<sub>2</sub> measurements. The diffusivity (Section 2.2.2) and soil flux across different soil layers (Section 2.2.3) are then computed.

The final step is computing a surface soil flux through extrapolation to the surface (purple parallelogram in Figure 1 and Panel c in Figure 2). Uncertainty on a soil flux measurement is computed through quadrature. An aggregate quality assurance (QA) flag for each environmental measurement is also reported, representing if any gap-filled measurements were used in the computation of a soil flux. Within the soil flux-gradient method, several different approaches can be used to derive a surface flux (Maier & Schack-Kirchner, 2014); the `neonSoilFlux` package reports eight different possible values of soil surface flux (Section 2.2.3).

### 2.2.1 Gap-filling routine

NEON reports QA flags as a binary value for a given measurement and half-hourly time. We replaced any flagged measurements at a location's spatial depth  $z$  with a bootstrapped sample of the monthly mean for all un-flagged measurements for that month. These measurements are represented by the vector  $\mathbf{m}$ , standard errors  $\sigma$ , and the 95% confidence interval (the so-called expanded uncertainty, Farrance & Frenkel (2012))  $\epsilon$ . All of these vectors have length  $M$ . We have that  $\vec{\sigma}_i \leq \vec{\epsilon}_i$ . We define the bias as  $\mathbf{b} = \sqrt{\epsilon^2 - \sigma^2}$ .

We generate a vector of bootstrap samples of the distribution of the monthly mean  $\bar{m}$  and monthly standard error  $\bar{\sigma}$  the following ways:

1. Randomly sample from the uncertainty and bias independently:  $\sigma_j$  and the bias  $\mathbf{b}_k$  (not necessarily the same sample)
2. Generate a vector  $\mathbf{n}$  of length  $N$ , where  $\mathbf{n}_i$  is a random sample from a normal distribution with mean  $m_i$  and standard deviation  $\sigma_j$ . Since  $M < N$ , values from  $\mathbf{m}$  will be reused.
3. With these  $N$  random samples,  $\bar{y}_i = \bar{x} + \bar{b}_k$  and  $s_i$  is the sample standard deviation of  $\vec{x}$ . We expect that  $s_i \approx \vec{\sigma}_j$ .
4. The reported monthly mean and standard deviation are then computed  $\bar{\bar{y}}$  and  $\bar{s}$ . Measurements and uncertainties that did not pass the QA check are then substituted with  $\bar{\bar{y}}$  and  $\bar{s}$ .

### 2.2.2 Diffusivity computation

Soil diffusivity  $D_a$  at a given measurement depth is the product of the diffusivity in free air  $D_{a,0}$  ( $\text{m}^2 \text{s}^{-1}$ ) and the tortuosity  $\xi$  (no units) (Millington & Shearer, 1971). Surface barometric pressure (kPa) (National Ecological Observatory Network (NEON), 2024a), soil temperature at depth (National Ecological Observatory Network (NEON), 2024d), soil water content (National Ecological Observatory Network (NEON), 2024e), and soil physical properties (National Ecological Observatory Network (NEON), 2024c). Soil physical properties are surveyed once at each site, whereas the other measurements are provided on a half-hourly basis.

We compute  $D_{a,0}$  with Equation 1:

$$D_{a,0} = 0.0000147 \cdot \left( \frac{T_i + 273.15}{293.15} \right)^{1.75} \cdot \left( \frac{P}{101.3} \right) \quad (1)$$

where  $T_i$  is soil temperature ( $^{\circ}\text{C}$ ) at depth  $i$  (National Ecological Observatory Network (NEON), 2024d) and  $P$  surface barometric pressure (kPa) (National Ecological Observatory Network (NEON), 2024a). At that soil depth, the tortuosity  $\xi$  is defined by Equation 2 (Millington & Shearer, 1971):

$$\xi = \frac{(\phi - SWC_i)^{10/3}}{\phi^2} \quad (2)$$

In Equation 2,  $SWC$  is the soil water content at depth  $i$  (National Ecological Observatory Network (NEON), 2024e) and  $\phi$  is the porosity (Equation 3), which in turn is a function of soil physical properties (National Ecological Observatory Network (NEON), 2024c).

The tortuosity  $\xi$  is computed from soil porosity  $\phi$ . :

$$\phi = \left(1 - \frac{\rho_s}{\rho_m}\right) (1 - f_V) \quad (3)$$

In Equation 3,  $\rho_m$  is the particle density of mineral soil (2.65 g cm<sup>-3</sup>),  $\rho_s$  the soil bulk density (g cm<sup>-3</sup>) excluding coarse fragments greater than 2 mm (National Ecological Observatory Network (NEON), 2024c). The term  $f_V$  is a site-specific value that accounts for the proportion of soil fragments between 2-20 mm. Soil fragments greater than 20 mm were not estimated due to limitations in the amount of soil that can be analyzed (National Ecological Observatory Network (NEON), 2024c). We assume there are no pores within rocks. Values of  $\rho_s$ ,  $\rho_m$  are assumed to be constant across the soil profile and the same at each site sampling location.

### 2.2.3 Soil flux computation

We applied Fick's law (Equation 4) to compute the soil flux  $F_{ij}$  ( $\mu\text{mol m}^{-2} \text{s}^{-1}$ ) across two soil depths  $i$  and  $j$ :

$$F_{ij} = -D_a \frac{dC}{dz} \quad (4)$$

where  $D_a$  is the diffusivity ( $\text{m}^2 \text{s}^{-1}$ ) and  $\frac{dC}{dz}$  is the gradient of  $\text{CO}_2$  molar concentration ( $\mu\text{mol m}^{-3}$ , so the gradient has units of  $\mu\text{mol m}^{-3} \text{m}^{-1}$ ). The diffusivity (described below) is a function of soil temperature, soil water content, and soil physical properties. The soil surface flux is theoretically defined by applying Equation 4 to measurements collected at the soil surface and directly below the surface. Measurements of soil temperature, soil water content, and soil  $\text{CO}_2$  molar concentration across the soil profile allow for application of Equation ?? across different soil depths. The flux gradient method approximates the soil surface flux either by (1) computation Equation 4 across sub-surface measurement depths to the surface. Each site had three measurement layers, so we denote the flux between which two layers as a three-digit subscript  $F_{ijk}$  where indicator variables indicating if a given layer was used (written in order of increasing depth), according to the following:



- $F_{000}$  is a surface flux estimate using the intercept of the linear regression of  $D_a$  and the slope from linear regression of  $\text{CO}_2$  (which represents  $\frac{dC}{dz}$  in Fick's Law). Tang et al. (2003) used this approach to compute fluxes in an oak-grass savannah.
- $F_{110}$ ,  $F_{011}$  are fluxes across the two most shallow layers and two deepest layers respectively. The diffusivity used in Fick's Law is always at the deeper measurement layer. When used as a surface flux estimate we assume  $\text{CO}_2$  remains constant above this flux depth.
- $F_{101}$  is a surface flux estimate using linear extrapolation using concentration measurements between the shallowest and deepest measurement layer. Hirano et al. (2003) and Tang et al. (2005) used an approach similar to  $F_{101}$  in a temperate deciduous broadleaf forest and ponderosa pine forest respectively.

Uncertainty in all  $F_{ijk}$  is computed through quadrature.

## 2.3 Post processing evaluation

Following collection of field measurements from the LICOR and calculation of the soil fluxes from `neonSoilFlux` package, we compared measured soil fluxes (from the LICOR instruments) to a given soil flux calculation during the same half hour. At each site and flux computation method we also computed the  $R^2$  value for the half-hourly and measured LICOR values and the RMSE.

We evaluate the efficacy of results from the flux-gradient method in two ways. First, we calculated the signal to noise ratio (SNR), defined as the ratio of the reported flux to its uncertainty ( $F_{ijk}/\sigma_{ijk}$ ).

We evaluated if the measured field fluxes were within the calculated uncertainty from the flux-gradient method using the various approaches outlined above. We observed that the calculated quadrature uncertainty in many cases can be much larger than the reported measurement (as shown through the signal to noise ratio,  $\text{SNR} = F_{ijk}/\sigma_{ijk}$ ). We evaluated  $|F_S - F_{ijk}| < (1-\epsilon)\sigma_{ijk}$ , where  $F_S$  is a measured field soil flux from the LICOR 6800 (the LICOR 8250 was used at only three sites) and  $F_{ijk}$  is a computed flux method from the flux-gradient, and  $\sigma_{ijk}$  is the reported uncertainty for the flux method. The parameter  $\epsilon$  was an uncertainty reduction factor to evaluate how sensitive the results were given, measured by the proportion of field measurements contained in that range.

## 2.4 Diffusivity back calculations

We also computed the diffusivity at each of the different sites from the derived flux values and the reported gradient in  $\text{CO}_2$  at each of the surface layers (Figure XXXX) through dividing  $F_{field}/dC/dz$ . These values were then compared to reported diffusivity from the flux computation method.

Finally, the bulk density at a given site was then also computed through back calculation.

### 3 Results

Figure 3 reports out the measured fluxes from the LICOR 6800 and 8250 and computed fluxes and uncertainty at each measurement site. Results are reported in local time. Positive values of the flux indicate that there is a flux moving towards the surface. For ease of clarity the fluxes at  $F_{111}$  and  $F_{000}$  are only shown in the top row (surface), followed by the fluxes at individual separate layer ( $F_{100}$ ,  $F_{010}$ ,  $F_{001}$ ). Overall, with the exception of WREF and SRER (discussed later) the computed fluxes were on the same order of magnitude and timing as the measured field fluxes.

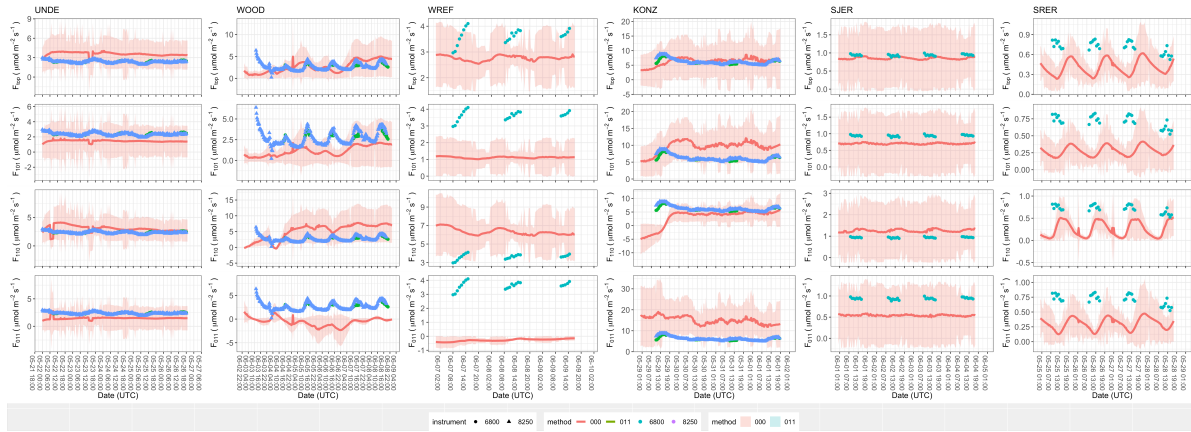


Figure 3: Results for different flux computations, organized by site (in increasing temperature shown at each site) across different measurement levels.  $F_{000}$  comes from the diffusivity extrapolation and  $F_{111}$  extrapolation across the surface. Field measurements are shown at the top of each plot. The computed flux values are shown with reported uncertainty as well.

Figure 4 reports the usage of gap-filled environmental measurement types (which could be one  $\text{CO}_2$ ,  $\text{SWC}$ , or  $T_s$  at any measurement depth, and also including  $P$ ) to compute  $F_s$ . Panel a) reports the proportion of gap-filled values for an environmental measurement at each site and Panel b) displays the distribution of gap-filled measurements at each site. The largest contribution to gap-filled measurements was soil water. SJER and WOOD utilized the largest number of gap-filled measurements, which were primarily  $\text{SWC}$  and  $T_s$ .

Figure: flux results at the different levels (000,111,001,010,100) Diffusivity at the different levels for comparison (also include derived diffusivity?) Stats at the different levels (with the lags)

LEAD IN TABLE HERE These results are reported in Figure 6.

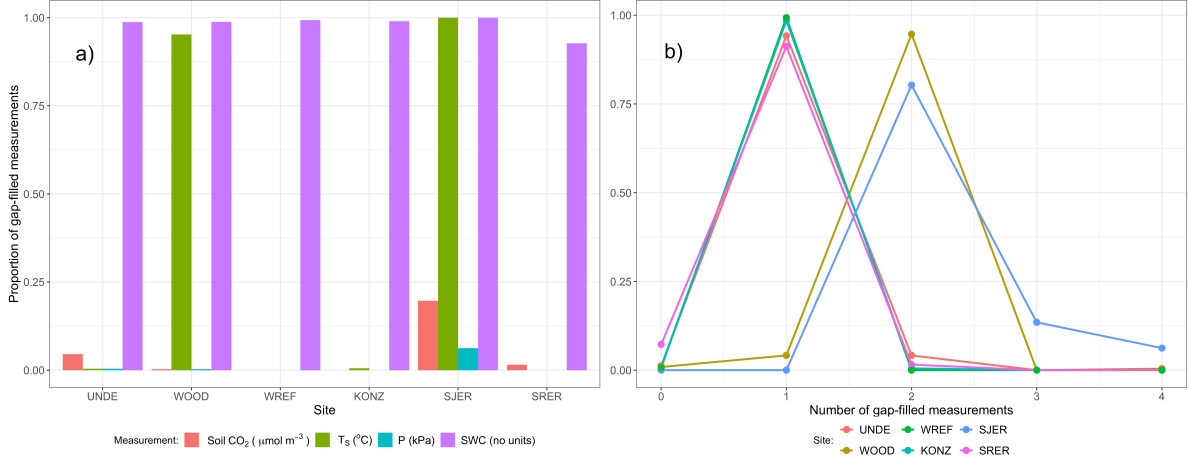


Figure 4: Panel a) Proportion of gap-filled environmental measurements used to generate  $F_S$  from the `neonSoilFlux` package, by study site. Panel b) distribution of the usage of gap-filled measurements at each site.

Calculated diffusivity from both the `neonSoilFlux` method and back calculated from the LI-COR are reported in Figure Figure 7. SAY MORE

## 4 Discussion

This study presents a unified data science workflow to efficiently process automated measurements of belowground soil CO<sub>2</sub> concentrations, water, and temperature to infer estimates of soil surface CO<sub>2</sub> effluxes through application of Fick's Law (Equation XXX). Our core goals in this study were: (1) to generate estimates of soil flux from continuous soil sensor data at terrestrial NEON sites using the flux-gradient method and then (2) to compare those estimates to field-measured fluxes based on the closed chamber approach at six NEON focal sites. We here discuss our progress toward these core goals through (1) an overall evaluation of the flux-gradient approach (and uncertainty calculation) and (2) site-specific evaluation of differences in estimated vs measured fluxes.

### 4.1 General evaluation of flux-gradient approach

Key assumptions of the flux-gradient approach are that CO<sub>2</sub> concentrations increase throughout the soil profile. We found that this condition was met at XXX% across the study period. Periods where this gradient condition are not met generally are connected to biophysical processes such soil wetting events (e.g. KONZ), which have the effect of temporarily reducing the soil respiration or efflux. For modeling soil respiration, typically a non-linear response function is considered, that also considers soil type as well (Bouma & Bryla, 2000; Yan et al.,

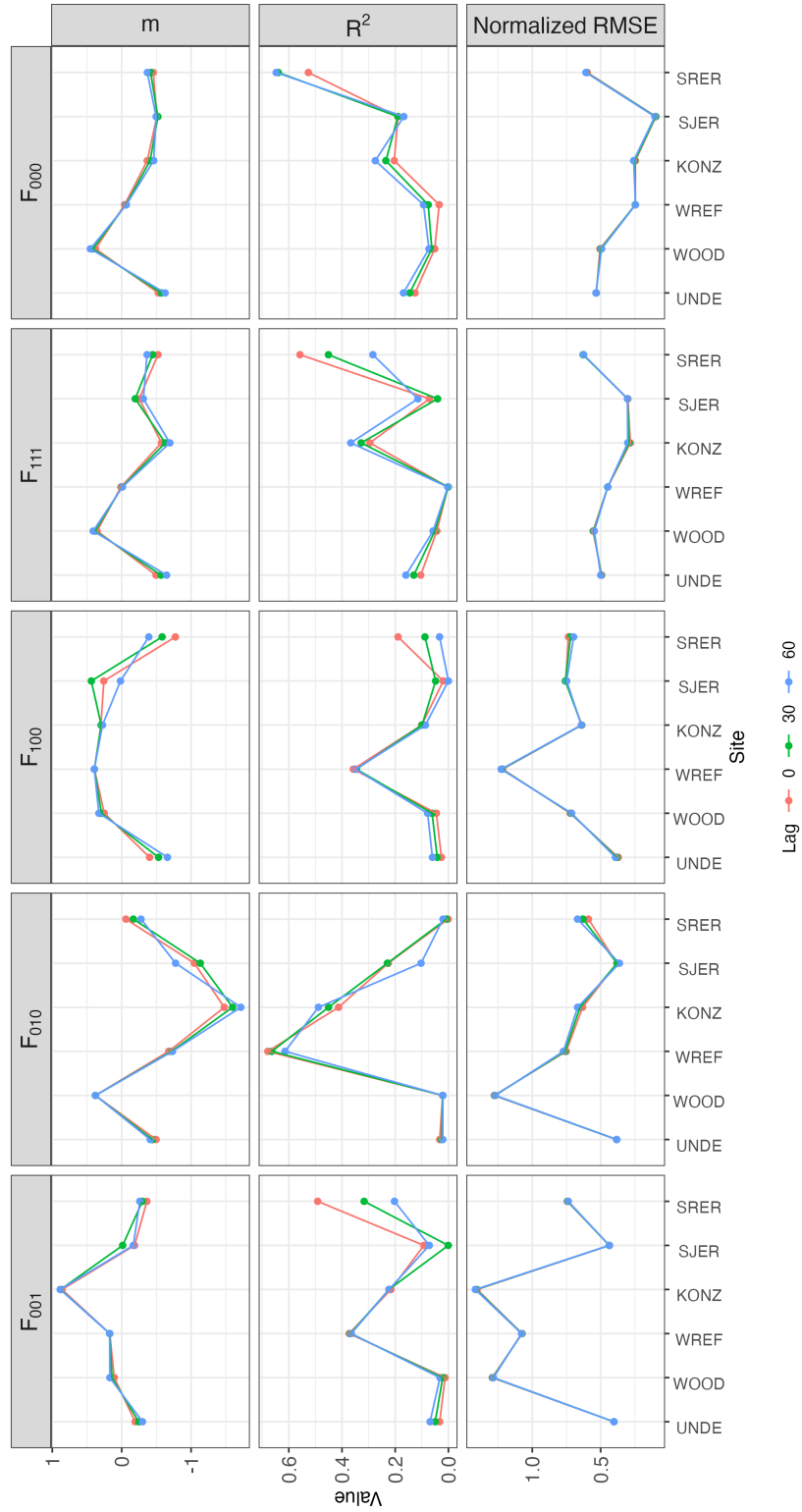


Figure 5

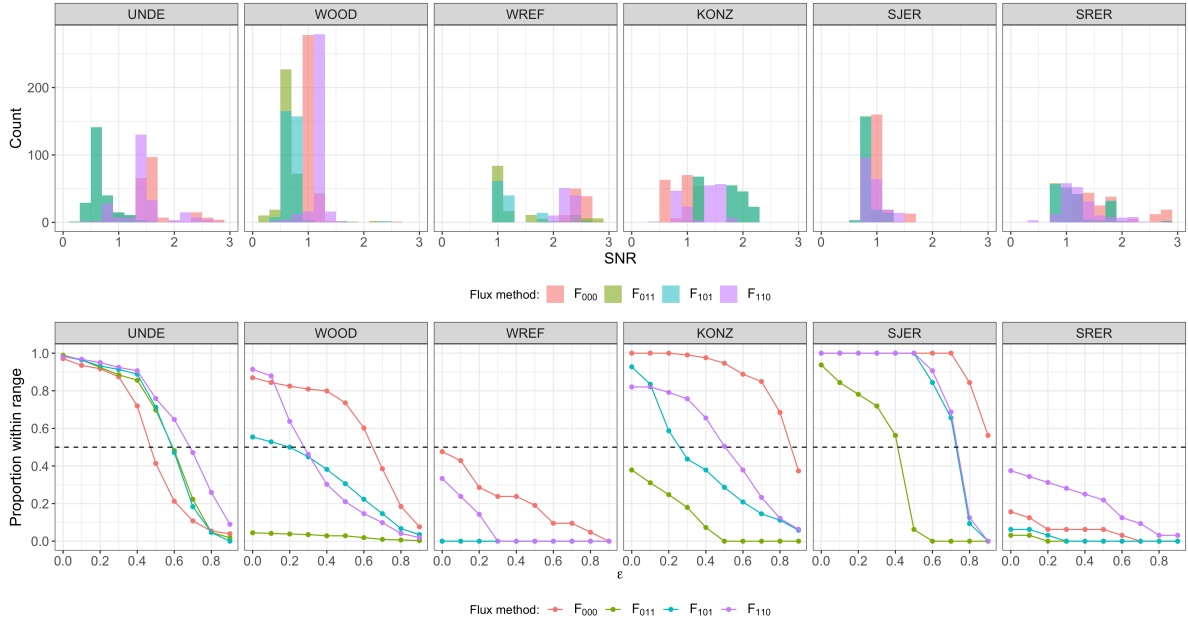


Figure 6: Top panel: distribution of SNR values across each of the different sites for the  $F_{000}$  and  $F_{111}$  flux gradient calculations. Bottom panel: Computation of uncertainty reduction to evaluate. As  $\epsilon$  increases this indicates that the uncertainty estimate reduces, making it harder to be within the range. SAY MORE

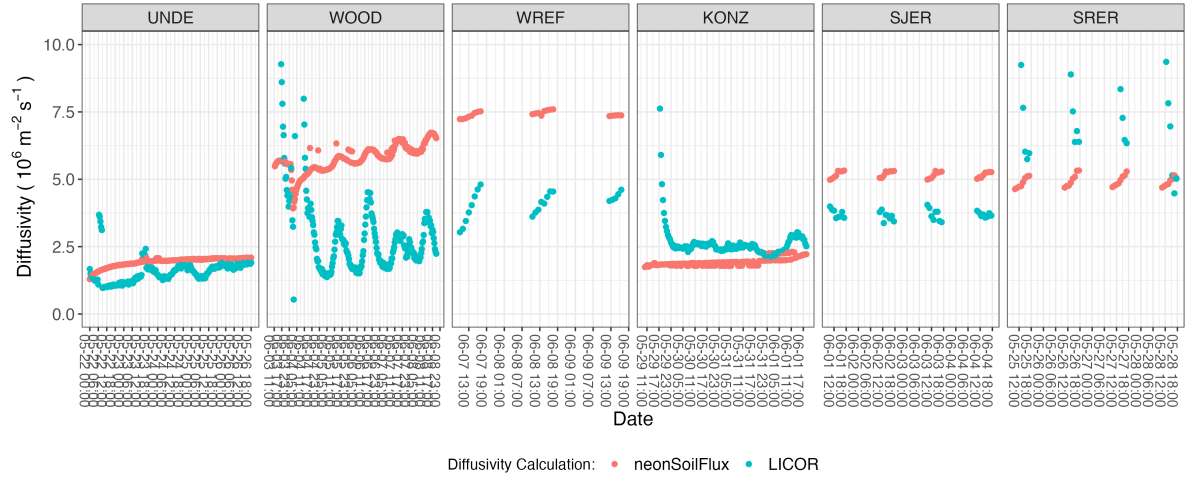


Figure 7: Calculation of diffusivity at each of the sites SAY MORE

2016, 2018). For the `neonSoilFlux` package soil type is connected to the bulk density, which is separately determined / measured at a site.

The largest source of uncertainty to improve reliability of the flux estimate is to prevent the usage of gap-filled data, especially with soil water (Figure XXX). Across the observed half-hourly periods for field measurements, the percentage of half-hourly periods where all four environmental measurements were available spanned from 0% (SJER) to 7% (SRER), but three sites (WREF, SRER, UNDE) had 95% of half-hourly intervals with just one gap-filled measurement. Where appropriate we have replaced measurements flagged to the protocol with a monthly gap-filled value. Further extensions of the gapfilling method could use more sophisticated gap-filling routines, similar to what is used for net ecosystem carbon exchange (Falge et al., 2001; Liu et al., 2023; Mariethoz et al., 2015; Moffat et al., 2007; Zhang et al., 2023).

Diffusivity taken from the megapit. Big microsite and temporal differences, soil shrink / swell. How do we think about what that means for using this approach to generalize across a NEON site over continuous time.

- Back calculation of bulk density to NEON sites (boxplot figure).

## 4.2 Evaluation of flux-gradient approach at each site

The six sites studied provide separate case studies for considerations when applying the flux-gradient method to evaluate resulting uncertainties and fluxes.

SRER is characterized by sandy soil, which also led to the hottest site there. Fluxes are driven by the change and response to temperature in the temperature driven, whereas we observed a decoupling of temperature across the different layers (supplementary figures?) For this instance, using the flux across the top two layers ( $F_{110}$ ) produced a pattern of soil flux consistent with the observed field data. The remaining methods  $F_{101}$ ,  $F_{011}$ , or  $F_{000}$  are derived from information at the deeper layer, which is decoupled both in terms of temperature and  $\text{CO}_2$  concentration.

KONZ is a site that experienced a significant rain event prior to sampling with eventual drying out over the course of the experiment. In this case we observed storage of soil water (as shown in supplementary figures), which increased the soil  $\text{CO}_2$  at the top layer, leading to negative values of flux at the start of the experiment, with the fluxes drying out afterwards. In this case only when the soil dried out (or returned to a baseline level), that the fluxes at the provided layer would work out in this case.

WREF experienced an extreme rainfall event in the days preceding field measurements, which meant that flux estimates calculated during the field measurement period sensors relied of gap-filled data. In this case,  $F_{000}$  is the better one.

We were able to show that the flux-gradient method produced estimates within XX of the field measured values at X of Y sites.

Tang et al. (2003) noticed a similar pattern in temperature as SRER. Mention alternative diffusivity calculations? (Sallam - but this may not be a factor compared to water availability and gap filling)

When considering systematic deployment of this method across a measurement network, we faced a number of independent challenges for consideration. In developing and validating our approach, we faced a number of challenges related to data availability, including... gap filling, sensor calibration, depth interpolation, rainstorms, etc These errors are all

Derived results from the `neonSoilFlux` package have patterns that are consistent, and comparable, to those directly measured to the field (Figure XXX). The advantage to the `neonSoilFlux` package is the calculation of fluxes across different measurement depths, allowing for additional site-specific customization. Here application of the flux-gradient method provides a baseline estimate of soil fluxes that could be complemented through additional field measurements (e.g. LI-COR).

### 4.3 Recommendations for future method development

The `neonSoilFlux` package provides three different approaches of values for a soil flux. We believe these approaches reflect a variety of site-specific determination and assumptions used to generate a soil flux measurement (Maier & Schack-Kirchner, 2014), with the choice of method having a determinative approach on reported values. Reported results could further be distilled down using ensemble averaging approaches (Elshall et al., 2018; Raftery et al., 2005).

Figures XXX suggests that the provided uncertainty from `neonSoilFlux` is an overestimate compared to what is actually computed. When  $\epsilon = 0$  in Figure Figure 6, that means we are just using the reported uncertainty from `neonSoilFlux`. Looking at that (epsilon = 0) shows field measurements UNDE, KONZ, SJER are 100% within the reported intervals from `neonSoilFlux`. But those sites tend to have a  $SNR < 1$ , so the uncertainty is pretty noisy. For UNDE, we could even reduce the uncertainty by a factor of 75% (epsilon = 0.75), more than half of the field measurements will still be within the reported intervals. For KONZ, we are still within 70% of the reported intervals when uncertainty is reduced by 90%. That suggests that while the reported accuracy (as compared to field measurements), we do have higher precision.

These challenges notwithstanding, the method used here and made available in the `neonSoilFlux` R package is able to produce nearly continuous estimates of flux across all XXYY terrestrial NEON sites. These estimates are a significant improvement on available approaches to constrain the portion of ecosystem respiration attributable to the soil. This, in

turn, aids in our ability to understand the components of net ecosystem flux assessed at these sites using the co-located eddy flux towers.

- Refine estimates to provide a realistic constraint on surface concentration measurements, thereby increasing the gradient.
- Apply machine learning algorithms (e.g. random trees) or model averaging techniques to generate a single flux estimate across each sites spatial location
- Benchmarking flux results to estimates provided by Net ecosystem carbon exchange.

## 5 Conclusions

We have here presented an R package `neonSoilFlux` for the estimation of soil CO<sub>2</sub> fluxes from continuous buried soil sensor measurements across terrestrial National Ecological Observatory Network sites. We compared the predicted fluxes to those measured directly using a field-based closed chamber approach. We find that...

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## 7 Conflict of Interest Statements

None declared.

## 8 Author Contributions

Review and compile author credit statements from Google sheet.

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