

1 A direct comparison between field-measured

2 and sensor-based estimates of soil carbon

3 dioxide flux across six National Ecological

4 Observatory Network sites enabled by the

5 neonSoilFlux R package

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²¹ **Conflict of Interest Statements**

²² None of the authors have a financial, personal, or professional conflict of interest related to
²³ this work.

²⁴ **Author Contributions**

²⁵ Conceptualization: JZ, NZ; Methodology: EA, JZ, NZ; Software: JZ, NZ, ZW, E A, DM, RA,
²⁶ LX, LL; Validation: JZ, NZ; Formal Analysis: JZ, NZ, DM, RA, LX, LL; Investigation: JZ,
²⁷ NZ, RF-S, CT, NA-W, LB; Resources: JZ, NZ; Data curation: JZ, NZ, DM, LX; Writing
²⁸ – original draft: JZ, NZ; Writing – review and editing: JZ, NZ, ZW, EA, CT, DM, LX,;
²⁹ Visualization: JZ, NZ, DM, RA, LX; Supervision: JZ; NZ; Project Administration: JZ; NZ;
³⁰ Funding Acquisition: JZ; NZ

³¹ **Data Availability**

³² Data available from the Zenodo LINK <http://dx.doi.org/10.5061/dryad.41qh7> (Kiere & Drummond 2016)."

³⁴ **1 Abstract**

³⁵ A key component of constraining the uncertainty of the terrestrial carbon sink is quantification
³⁶ of terrestrial soil carbon fluxes, which vary across time and ecosystem type. One method for
³⁷ the estimation of these fluxes and their associated uncertainties is the flux gradient method,
³⁸ which can be calculated via a variety of existing approaches. Robust estimation of soil carbon
³⁹ fluxes on a sub-daily level requires measurements of soil CO₂ concentration, water content,
⁴⁰ temperature, and other environmental measurements and soil properties. These data are
⁴¹ publicly available from the National Ecological Observatory Network at sites spanning a range
⁴² of 20 different ecoclimatic domains across the continental United States, Puerto Rico, Alaska,
⁴³ and Hawai'i. We present an R software package (`neonSoilFlux`) that acquires NEON soil
⁴⁴ environmental data and computes soil carbon flux at a half-hourly time step at a user-specified
⁴⁵ NEON site and month in a tidy data format. To validate the computed fluxes, we visited six
⁴⁶ focal NEON sites and measured soil carbon fluxes using a closed-dynamic chamber approach.
⁴⁷ The validation confirmed that a primary challenge in reducing soil carbon flux uncertainty is
⁴⁸ correctly characterizing diffusivity and soil water content across the soil profile. Outputs from
⁴⁹ the `neonSoilFlux` package contribute to existing databases of soil carbon flux measurements,
⁵⁰ providing near real-time estimates of a critical component of the terrestrial carbon cycle.

⁵¹ **1.1 Keywords**

⁵² Soil carbon, carbon dioxide, flux gradient, carbon cycle, field validation, soil respiration, ecosys-
⁵³ tem variability, diffusion

⁵⁴ **2 Data for peer review**

⁵⁵ Anonymous data and code for peer review is available here: [LINK](#)

⁵⁶ **3 Introduction**

⁵⁷ Soils contain the largest reservoir of terrestrial carbon (Jobbágy & Jackson, 2000). A critical
⁵⁸ component of this reservoir is soil organic matter, the accumulation of which is influenced
⁵⁹ by biotic factors such as above-ground plant inputs (Jackson et al., 2017). These inputs in
⁶⁰ turn are influenced by environmental factors such as growing season length, temperature, and
⁶¹ moisture (Desai et al., 2022), which also affect the breakdown of soil organic matter and its
⁶² return to the atmosphere. Across heterogeneous terrestrial landscapes, the interplay between
⁶³ these biotic and abiotic factors influence the size of the soil contribution to the terrestrial
⁶⁴ carbon sink (Friedlingstein et al., 2023). However, the heterogeneity of these processes across
⁶⁵ diverse ecosystems in the context of rapid environmental change leads to large uncertainty in
⁶⁶ the magnitude of this sink in the future, and thus a pressing need to quantify changes in soil
⁶⁷ carbon pools and fluxes across scales.

⁶⁸ Ecological observation networks such as the United States' National Ecological Observatory
⁶⁹ Network (NEON) and others (e.g. FLUXNET or the Integrated Carbon Observation System)
⁷⁰ present a significant advancement in the nearly continuous observation of biogeochemical pro-
⁷¹ cesses at the continental scale. Notably, at 47 terrestrial sites across the continental United
⁷² States, NEON provides half-hourly measurements of soil CO₂ concentration, temperature,
⁷³ and moisture at different vertical depths. Each of these NEON sites also encompasses mea-
⁷⁴ surements of the cumulative sum of all ecosystem carbon fluxes in an airshed using the eddy
⁷⁵ covariance technique (Balderuppi, 2014). Soil observations provided by NEON are on the same

76 timescale and standardized with eddy covariance measurements from FLUXNET. These types
77 of nearly continuous observational data (NEON and FLUXNET) can be used to reconcile dif-
78 ferences between model-derived or data-estimated components of ecosystem carbon flux (Jian
79 et al., 2022; Luo et al., 2011; Phillips et al., 2017; J. Shao et al., 2015; P. Shao et al., 2013;
80 Sihi et al., 2016).

81 Estimated or observed soil carbon fluxes are a key metric for understanding change in soil
82 carbon pools over time (Bond-Lamberty et al., 2024). A soil carbon flux to the atmosphere
83 (F_S , units $\mu\text{mol m}^{-2} \text{s}^{-1}$), represents the aggregate process of transfer of soil CO_2 to the
84 atmosphere from physical and biological processes (e.g. diffusion and respiration). Soil carbon
85 fluxes can be assumed to encompass soil carbon respiration from autotrophic or heterotrophic
86 sources (Davidson et al., 2006), typically assumed to be static across the soil biome and
87 modeled with a exponential Q_{10} paradigm (Bond-Lamberty et al., 2004; Chen & Tian, 2005;
88 Hamdi et al., 2013).

89 One method by which F_S is measured in the field is through the use of soil chambers in a closed,
90 well-mixed system (Norman et al., 1997) with headspace trace gas concentrations measured
91 with an infrared gas analyzer (IRGA). F_S can also be estimated from soil CO_2 measurements
92 at different depths in the soil using the flux-gradient method (Maier & Schack-Kirchner, 2014).
93 This method is an approach that uses conservation of mass to calculate flux at a vertical soil
94 depth z at steady state by applying Fick's law of diffusion. A simplifying assumption for the
95 flux-gradient method is that there is no mass transfer in the other spatial dimensions x and y
96 (Maier & Schack-Kirchner, 2014). The diffusivity profile, a key component of this calculation,
97 varies across the soil depth as a function of soil temperature, soil volumetric water content,
98 atmospheric air pressure, and soil bulk density (Millington & Shearer, 1971; Moldrup et al.,
99 1999; Sallam et al., 1984).

100 Databases such as the Soil Respiration Database (SRDB) or the Continuous Soil Respiration

101 Database (COSORE) add to the growing network of resources for making collected observa-
102 tions of soil fluxes available to other workers (Bond-Lamberty, 2018; Bond-Lamberty et al.,
103 2020; Bond-Lamberty & Thomson, 2010; Jian et al., 2021; Jiang et al., 2024). However, these
104 databases currently encompass primarily direct soil measurements of fluxes (i.e. those using
105 methods like the closed-chamber method described above). Currently, NEON provides all
106 measurements to calculate F_S from Fick's law, but soil flux as a derived data product was
107 descoped from the initial network launch due to budget constraints (Berenbaum et al., 2015).
108 Deriving estimates of F_S using continuous sensor data across NEON sites thus represents a
109 high priority.

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

114 Key objectives of this study are to:

- 115 1. Apply the flux-gradient method to estimate soil CO₂ flux from continuous sensor mea-
116 surements across NEON sites.
- 117 2. Benchmark estimated soil carbon fluxes against field measurements (e.g. direct chamber
118 measurements of soil flux).
- 119 3. Identify sources of error in the flux-gradient approach across diverse sites in order to
120 guide future work.

₁₂₁ **4 Materials and Methods**

₁₂₂ **4.1 Field methods**

₁₂₃ **4.1.1 Focal NEON Sites**

₁₂₄ In order to acquire field data to validate model predictions of flux, we selected six terrestrial
₁₂₅ NEON sites for analysis. We conducted field measurement campaigns at these sites, which
₁₂₆ span a range of environmental gradients and terrestrial domains (Table 1). SJER, SRER, and
₁₂₇ WREF were visited during May and June of 2022, and WOOD, KONZ, and UNDE during
₁₂₈ May and June of 2024.

₁₂₉ Over the course of two field campaigns in 2022 and 2024, we conducted week-long visits at
₁₃₀ each site. In consultation with NEON field staff, we first selected a specific plot in the soil
₁₃₁ sampling array to maximize the concurrent availability of sensor data.

₁₃₂ **4.1.2 Soil collar placement**

₁₃₃ Either one (2022 sampling campaign) or two (2024 sampling campaign) PVC soil collars (20.1
₁₃₄ cm inside diameter) were installed in close proximity to the permanent NEON soil sensors at
₁₃₅ each site (Figure 1). The soil plot where measurements were taken was chosen at each site
₁₃₆ in consultation with NEON staff to maximize likelihood of quality soil sensor measurements
₁₃₇ during the duration of the IRGA measurements at each site. After installation, collar(s) were
₁₃₈ left to equilibrate for approximately 24 hours prior to measurements being taken.

¹³⁹ **4.1.3 Infrared gas analyzer measurements of soil CO₂ flux**

¹⁴⁰ In 2022, we then made measurements of flux on an hourly interval for 8 hours each day.
¹⁴¹ Measurements were taken from roughly 8 am to 4 pm, with the time interval selected to
¹⁴² capture the majority of the diurnal gradient of soil temperature each day. These measurements
¹⁴³ were made using a LI-6800 infrared gas analyzer instrument (LI-COR Environmental, Lincoln,
¹⁴⁴ NE) fitted with a soil chamber attachment (attachment 6800-09). In 2024, we again used
¹⁴⁵ the same LI-6800 instrument, but made half-hourly measurements over an approximately 8
¹⁴⁶ hour period. In addition, we also installed a second collar and used a second instrument, an
¹⁴⁷ LI-870 CO₂ IRGA, connected to an automated robotic chamber (LI-COR chamber 8200-104)
¹⁴⁸ controlled by an LI-8250 multiplexer, to make automated measurements. The multiplexer was
¹⁴⁹ configured to take half-hourly measurements 24 hours a day for the duration of our sampling
¹⁵⁰ bout at each site. Each instrument was paired with a soil temperature and moisture probe
¹⁵¹ (Stevens HydraProbe, Stevens Water, Portland, OR) that was used to make soil temperature
¹⁵² and moisture measurements concurrent with the CO₂ flux measurements. Chamber volumes
¹⁵³ were set by measuring collar offsets at each site. System checks were conducted daily for the
¹⁵⁴ LI-6800 and weekly for the LI-8250. Instruments were factory calibrated before each field
¹⁵⁵ season.

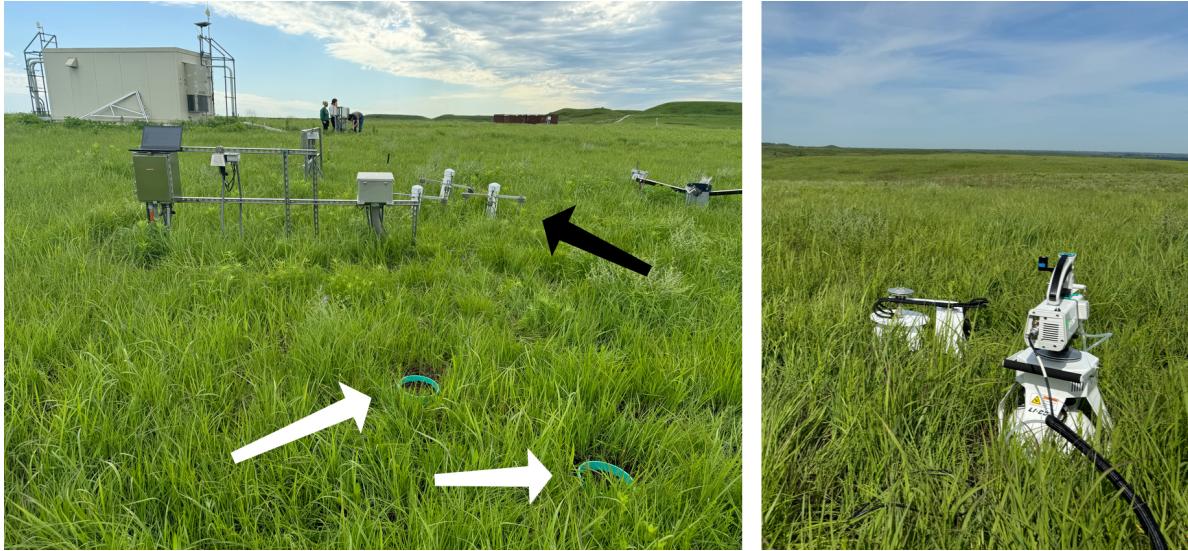


Figure 1: Spatial layout of field sampling using a closed-dynamic chamber setup at a representative NEON site (KONZ). Left image shows collars (white arrows) and permanent soil sensor installation (black arrow) and right image shows the LI-6800 (foreground) and LI-8200-104 (background) instruments placed on the collars.

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. Soil plot refers to the particular location in the soil sensor array (denoted as HOR by NEON) where field measurements were made.

Site (NEON site ID)	Location	Ecosystem type	Mean annual tempera- ture	$\overline{T_S}$ (°)	Mean annual precipita- tion	\overline{SWC} (%)	Field measure- ment dates	Soil plot
Santa	31.91068,	Shrubland	19.3°C	47.6°	346 mm	4.0%	29 May	004
Rita	-						2024 - 01	
Experi- mental Range (SRER)	110.83549						June 2024	

Table 1: Listing of NEON sites studied for field work and analysis. \bar{T}_S : average soil temperature during field measurements. \bar{SWC} : average soil water content during field measurements. Soil plot refers to the particular location in the soil sensor array (denoted as HOR by NEON) where field measurements were made.

Site (NEON site ID)	Location	Ecosystem type	Mean annual tempera- ture	\bar{T}_S (°)	Mean annual precipita- tion	\bar{SWC} (%)	Field measure- ment dates	Soil plot
San Joaquin Experimental Range (SJER)	37.10878, -	Oak woodland	16.4°C	41.7°	540 mm	1.2%	01 June 2022 - 04	005
Experi- mental Range (SJER)	119.73228						June 2022	
Wind River Experimental Forest (WREF)	45.82049, -	Evergreen forest	9.2°C	15.3°	2225 mm	27.2%	07 June 2022 - 09	001
Chase Lake Wildlife Refuge (WOOD)	121.95191 47.1282, - 99.241334	Restored prairie	4.9°C	14.9°	495 mm	14.9%	03 June 2024 - 09	001
National Biological Station (KONZ)		grassland					June 2024	
Konza Prairie	39.100774, -	Tallgrass Prairie	12.4°C	23.4°	870 mm	23.4%	29 May 2024 - 01	001
	96.563075						June 2024	

Table 1: Listing of NEON sites studied for field work and analysis. \bar{T}_S : average soil temperature during field measurements. \bar{SWC} : average soil water content during field measurements. Soil plot refers to the particular location in the soil sensor array (denoted as HOR by NEON) where field measurements were made.

Site (NEON site ID)	Location	Ecosystem type	Mean annual tempera- ture	\bar{T}_S (°)	Mean annual precipita- tion	\bar{SWC} (%)	Field measure- ment dates	Soil plot
University of Notre Dame Environ- mental Research Center (UNDE)	46.23391, - 89.537254	Deciduous forest	4.3°	13.0°	802 mm	13.0%	22 May 2024 - 25 May 2024	004

4.1.4 Post-collection processing of field data

We used LI-COR SoilFluxPro software (v 5.3.1) to assess the data after collection and to inform sampling parameters. We checked appropriateness of dead band and measurement durations using built-in evaluation tools. Based on this, the deadband period was set for 30-40 seconds, depending on the site, and the measurement duration was 180 seconds with a 30 second pre-purge and a 30 second post-purge at most sites, and a 90 sec pre- and post-purge at sites with higher humidity due to recent precipitation events. We also assessed the R^2 of linear and exponential model fits to measured CO_2 to verify measurement quality.

¹⁶⁴ **4.2 neonSoilFlux R package**

¹⁶⁵ We developed an R package (`neonSoilFlux`; <https://CRAN.R-project.org/package=neonSoilFlux>)
¹⁶⁶ to compute half-hourly soil carbon fluxes and uncertainties from NEON data. The objective
¹⁶⁷ of the `neonSoilFlux` package is a unified workflow (Figure 2) for soil data acquisition and
¹⁶⁸ analysis that supplements the existing data acquisition R package `neonUtilities` (LINK TO
¹⁶⁹ BE ADDED AFTER PEER REVIEW).

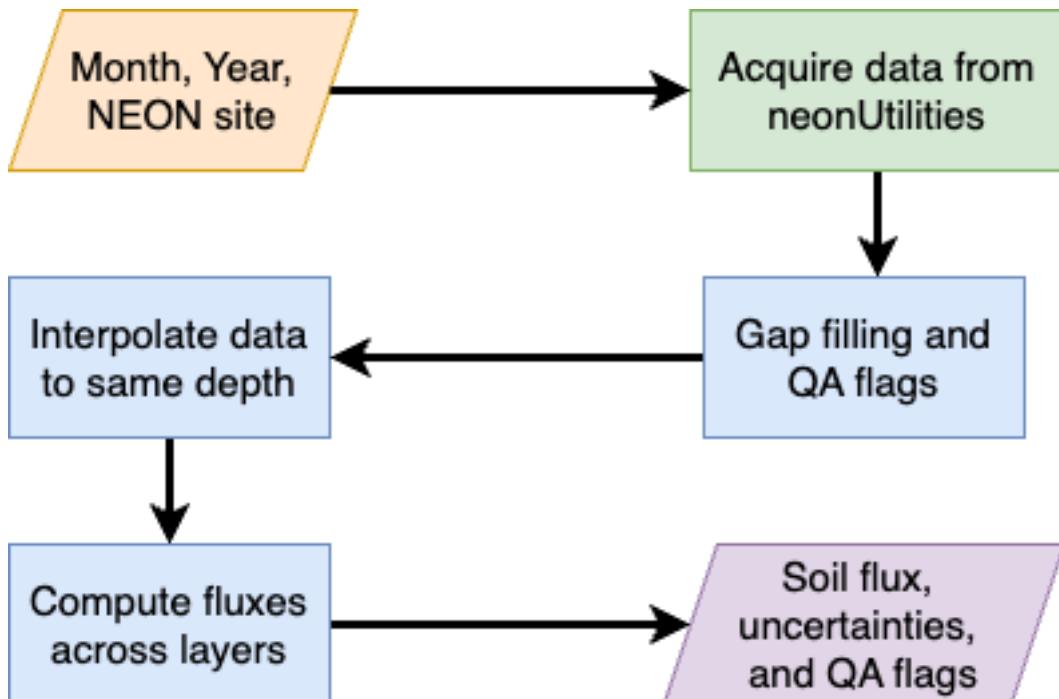


Figure 2: Diagram of `neonSoilFlux` R package. For a given month, year, and NEON site (orange parallelogram), the package acquires all relevant data to compute F_S using the `neonUtilities` R package (green rectangle). Data are gap-filled according to reported QA flags and interpolated to the same measurement depth before computing the soil flux, uncertainties, and final QA flags (blue rectangles). The package reports the associated soil flux, uncertainties, and quality assurance (QA) flags for the user (purple parallelogram).

¹⁷⁰ At a given NEON observation there are five replicate soil plots, each with measurements of
¹⁷¹ soil CO₂ concentration, soil temperature, and soil moisture at different depths (Figure 3). The

172 `neonSoilFlux` package acquires measured soil water content (National Ecological Observatory
 173 Network (NEON), 2024e), soil CO₂ concentration (National Ecological Observatory Network
 174 (NEON), 2024b), barometric pressure from the nearby tower (National Ecological Observa-
 175 tory Network (NEON), 2024a), soil temperature (National Ecological Observatory Network
 176 (NEON), 2024d), and soil properties (e.g. bulk density) (National Ecological Observatory Net-
 177 work (NEON), 2024c). The static soil properties were collected from a nearby soil pit during
 178 site characterization and are assumed to be constant at each site.

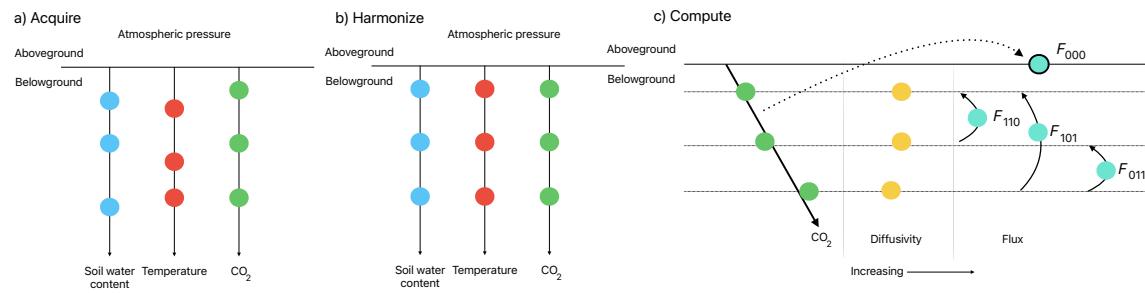


Figure 3: Model diagram for data workflow for the `neonSoilFlux` R package. a) Acquire: Data are obtained from given NEON location and horizontal sensor location, which includes soil water content, soil temperature, CO₂ concentration, and atmospheric pressure. All data are screened for quality assurance; if gap-filling of missing data occurs, it is flagged for the user. b) Any belowground data are then harmonized to the same depth as CO₂ 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 CO₂ with depth.

179 The workflow to compute a value of F_S with `neonSoilFlux` consists of three primary steps,
 180 illustrated in Figure 3. First, NEON data are acquired for a given site and month via the
 181 `neonUtilities` R package (yellow parallelogram and green rectangle in Figure 2 and Panel a
 182 in Figure 3). Acquired environmental data can be exported to a comma separated value file
 183 for additional analysis. Quality assurance (QA) flags are reported as an indicator variable.
 184 The second step is harmonizing the data to compute soil fluxes across soil layers. This step

185 consists of three different actions (blue rectangles in Figure 2 and Panel b in Figure 3). If a
186 given observation by NEON is reported as not passing a quality assurance check, we applied
187 a gap filling method to replace that measurement with its monthly mean at that same depth
188 (Section 4.2.1). Belowground measurements of soil water and soil temperature are then inter-
189 polated to the same depth as soil CO₂ measurements. The diffusivity (Section 4.2.2) and soil
190 flux across different soil layers (Section 4.2.3) are then computed.

191 The third and final step is computing a surface soil flux through extrapolation to the sur-
192 face (purple parallelogram in Figure 2 and Panel c in Figure 3). Uncertainty on a soil flux
193 measurement is computed through quadrature. An aggregate quality assurance (QA) flag
194 for each environmental measurement is also reported, representing if any gap-filled measure-
195 ments were used in the computation of a soil flux. Within the soil flux-gradient method,
196 several different approaches can be used to derive a surface flux (Maier & Schack-Kirchner,
197 2014); the `neonSoilFlux` package reports four different possible values for soil surface flux
198 (Section 4.2.3).

199 4.2.1 Gap-filling routine

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

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

- 208 1. Randomly sample from the uncertainty and bias independently: σ_j and the bias \mathbf{b}_k (not
 209 necessarily the same sample).
- 210 2. Generate a vector \mathbf{n} of length N , where \mathbf{n}_i is a random sample from a normal distribution
 211 with mean m_i and standard deviation σ_j . Since $M < N$, values from \mathbf{m} will be reused.
- 212 3. With these N random samples, $\bar{y}_i = \vec{x} + \vec{b}_k$ and s_i is the sample standard deviation of \vec{x} .
 213 We expect that $s_i \approx \vec{\sigma}_j$.
- 214 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
 215 $\bar{\bar{y}}$ and \bar{s} .

217 This gap-filling method described here provides a consistent approach for each data stream,
 218 however we recognize that other gap-filling alternatives may be warranted for longer-term gaps
 219 (e.g. such as correlations with other NEON measurement levels and soil plots), or measure-
 220 ment specific gap-filling routines. We discuss the effect of gap-filling on our measurements in
 221 Section 6.

222 **4.2.2 Soil diffusivity**

223 Soil diffusivity D_a at a given measurement depth is the product of the diffusivity in free air
 224 $D_{a,0}$ ($\text{m}^2 \text{ s}^{-1}$) and the tortuosity ξ (no units) (Millington & Shearer, 1971).

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

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

226 where T_i is soil temperature ($^{\circ}\text{C}$) at depth i (National Ecological Observatory Network
227 (NEON), 2024d) and P surface barometric pressure (kPa) (National Ecological Observatory
228 Network (NEON), 2024a).

229 Previous studies by Sallam et al. (1984) and Tang et al. (2003) demonstrated the sensitivity
230 of modeled F_S depending on the tortuosity model used to compute diffusivity. At low soil
231 water content, the choice of tortuosity model may lead to order of magnitude differences in
232 D_a , which in turn affect modeled F_S . The `neonSoilFlux` package uses two different models
233 for ξ , representing the extremes reported in Sallam et al. (1984). The first approach uses the
234 Millington-Quirk model for diffusivity, Equation 2 (Millington & Shearer, 1971):

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

235 In Equation 2, SWC is the soil water content at depth i (National Ecological Observatory
236 Network (NEON), 2024e) and ϕ is the porosity (Equation 3), which in turn is a function of
237 soil physical properties (National Ecological Observatory Network (NEON), 2024c):

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

238 In Equation 3, ρ_m is the particle density of mineral soil (2.65 g cm^{-3}), ρ_s the soil bulk density
239 (g cm^{-3}) excluding coarse fragments greater than 2 mm (National Ecological Observatory
240 Network (NEON), 2024c). The term f_V is a site-specific value that accounts for the proportion
241 of soil fragments between 2-20 mm. Soil fragments greater than 20 mm were not estimated
242 due to limitations in the amount of soil that can be analyzed (National Ecological Observatory
243 Network (NEON), 2024c). We assume there are no pores within rocks.

²⁴⁴ The second approach to calculate ξ is the Marshall model (Marshall, 1959), where $\xi = \phi^{1.5}$,
²⁴⁵ with ϕ defined from Equation 3.

²⁴⁶ **4.2.3 Soil flux computation**

²⁴⁷ We applied Fick's law (Equation 4) to compute the soil flux F_{ij} ($\mu\text{mol m}^{-2} \text{s}^{-1}$) across two
²⁴⁸ soil depths i and j :

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

²⁴⁹ where D_a is the diffusivity ($\text{m}^2 \text{s}^{-1}$) and $\frac{dC}{dz}$ is the gradient of CO₂ molar concentration
²⁵⁰ ($\mu\text{mol m}^{-3}$, so the gradient has units of $\mu\text{mol m}^{-3} \text{m}^{-1}$). The soil surface flux is theoretically
²⁵¹ defined by applying Equation 4 to measurements collected at the soil surface and directly
²⁵² below the surface. Measurements of soil temperature, soil water content, and soil CO₂ molar
²⁵³ concentration across the soil profile allow for application of Equation 4 across different soil
²⁵⁴ depths. Each site had three measurement layers, so we denote the flux between which two
²⁵⁵ layers as a three-digit subscript F_{ijk} with indicator variables i , j , and k indicate if a given
²⁵⁶ layer was used (written in order of increasing depth), according to the following:

- ²⁵⁷ • F_{000} is a surface flux estimate using the intercept of the linear regression of D_a with
²⁵⁸ depth and the slope from the linear regression of CO₂ with depth (which represents $\frac{dC}{dz}$
²⁵⁹ in Fick's Law). Tang et al. (2003) used this approach to compute fluxes in an oak-grass
²⁶⁰ savannah.
- ²⁶¹ • F_{110} , F_{011} are fluxes across the two most shallow layers and two deepest layers respec-
²⁶² tively. The diffusivity used in Fick's Law is always at the deeper measurement layer.

When used as a surface flux estimate we assume CO₂ 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 (Taylor, 2022).

4.3 Post processing evaluation

Following collection of field measurements and calculation of the soil fluxes from `neonSoilFlux` package, we compared measured F_S based on closed-dynamic chamber measurements with the LI-COR instruments to a given soil flux calculation from `neonSoilFlux` for each site and flux computation method. Statistics included the associated R² value, root mean squared error (RMSE), and signal to noise ratio (SNR), defined as the ratio of a modeled soil flux (F_{ijk}) from `neonSoilFlux` to its quadrature uncertainty (σ_{ijk}).

We observed that the range of values (e.g. $F_{ijk} \pm \sigma_{ijk}$) was much larger than the measured field flux. We evaluated $|F_S - F_{ijk}| < (1 - \epsilon)\sigma_{ijk}$, where F_S is a measured field soil flux from the LI-COR 6800 (as the LI-COR 870/8250 was used at only three sites in 2024 but the 6800 was used at all sites in both years). The parameter ϵ was an uncertainty reduction factor to evaluate how much the quadrature uncertainty could be reduced while maintaining precision between modeled F_{ijk} and measured F_S .

Finally, for a half-hourly interval we also computed a *post hoc* D_a using the LI-COR flux along with the CO₂ surface gradient reported by NEON using the measurement levels closest to the surface.

286 **5 Results**

287 Our overall goal was to design and validate an R package to estimate soil carbon dioxide
288 fluxes fluxes across terrestrial NEON sites using the flux gradient method. Validation of the
289 approach was based on comparison of estimated fluxes to field measurements made at six
290 focal sites. We first present our field measurement results, then the concordance between the
291 modeled and measured results, and lastly assess the factors that influenced the success of the
292 modeled approach at a given site.

293 **5.1 Field measurements**

294 We visited six NEON sites in the summers of 2022 and 2024. Using a closed-dynamic chamber
295 approach, we quantified soil carbon dioxide fluxes over the course of a week at each site. The
296 sites we visited ranged substantially in both their annual average temperature and precipitation
297 as well as their biome type (Table 2). These differences also influenced the wide range of
298 observed flux rates across sites. We used a LI-6800 to take manual hourly measurements at
299 the sites we visited in 2022 (SRER, SJER, WREF) and half-hourly manual measurements for
300 the sites we visited in 2024 (UNDE, KONZ, WOOD). In 2024 we also used an automated
301 chamber system (LI-870/LI-8250) to take half-hourly measurements 24 hours a day, thereby
302 also capturing nighttime fluxes in addition to the daytime fluxes also measured with the LI-
303 6800.

304 **5.2 Concordance between modelled and measured soil CO₂ flux**

305 The timeseries of the measured fluxes from the LI-COR 6800 and 870/8250 were compared
306 to modeled soil fluxes from the `neonSoilFlux` R package (Figure 4). We also assessed year-

Table 2: Summary of measured soil characteristics and flux results from field measurements across six NEON sites using a LI-COR 6800 (LI-870/8250 measurements omitted to enable direct comparability) via the closed-dynamic chamber method. Numeric values for soil CO₂ flux, soil temperature, and volumetric soil water content (VSWC) are the mean and standard deviation of field measurements at each site.

Site	Flux μmol m ⁻² s ⁻¹	Soil temp °C	VSWC cm ³ cm ⁻³	n
UNDE	2.55 ± 0.26	14.33 ± 0.77	0.33 ± 0.02	61
WOOD	3.02 ± 0.4	16.01 ± 1.54	0.28 ± 0.01	53
WREF	3.62 ± 0.3	15.34 ± 1.76	0.27 ± 0.06	21
KONZ	6.35 ± 0.97	27.28 ± 4.14	0.37 ± 0.01	44
SJER	0.94 ± 0.02	41.68 ± 11.22	0.01 ± 0.01	32
SRER	0.72 ± 0.09	47.64 ± 7.46	0.04 ± 0.01	32

307 long estimated flux time series and compared those to field measurements made at each site
308 (Figure 5). Results are reported in local time. Where applicable, sites are displayed from left
309 to right by increasing soil temperature (Table 1). Positive values of the flux indicate that there
310 is a flux moving towards the surface. Overall, with the exception of SRER (discussed later) the
311 computed fluxes determined using a variety of plausible methods spanned the field-measured
312 fluxes, but the specific flux-gradient method that best approximated field measurements varied
313 by site.

314 5.3 Assessment of data gaps

315 For a given half-hourly time period, the `neonSoilFlux` packages assigns a QA flag for a mea-
316 surement if more one values across all measurement depths uses gap-filled data (Section 4.2.1).
317 Panel a of Figure 6 reports the proportion of gap-filled data for all input environmental mea-
318 surements at each site during the period when field measurements were made. Soil fluxes are
319 computed from 4 different types of input measurements (T_S , SWC , P , and CO₂), any of which
320 could have a QA flag in a half-hourly interval. Panel b of Figure 6 displays at each site the

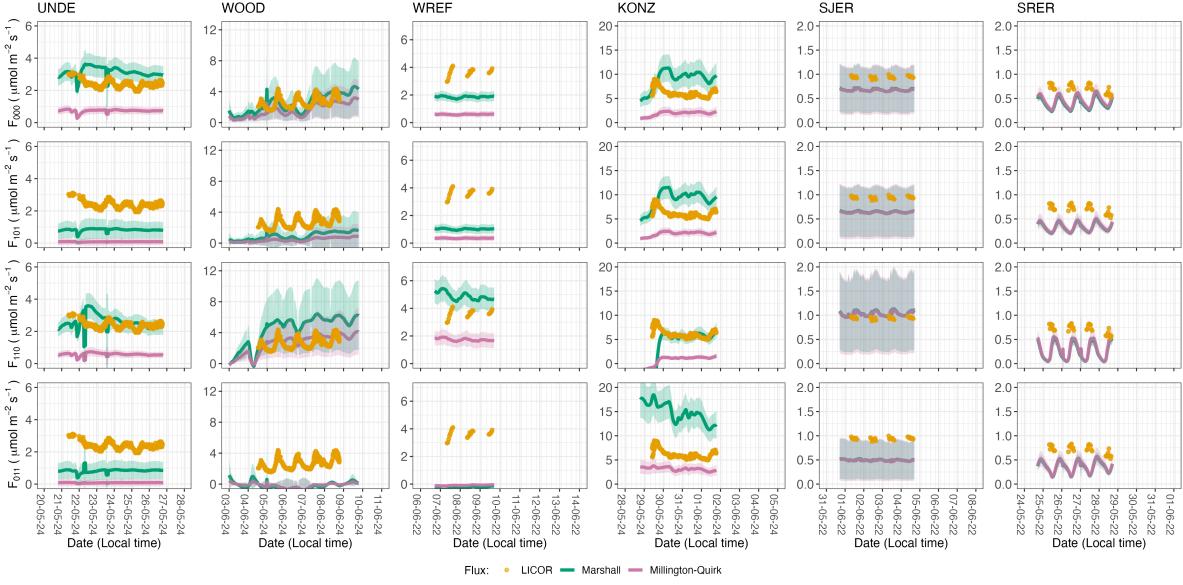


Figure 4: Timeseries of both measured F_S (yellow circles) and modeled soil fluxes (green or purple lines) by the `neonSoilFlux` R package. Fluxes from the `neonSoilFlux` R package are separated by the diffusivity model used (Millington-Quirk or Marshall, Section 4.2.2). Vertical axis labels in the first column represent the measurement levels where the flux-gradient approach is applied (Section 4.2.3). Ribbons for modeled soil fluxes represent ± 1 standard deviation. Results are reported in local time.

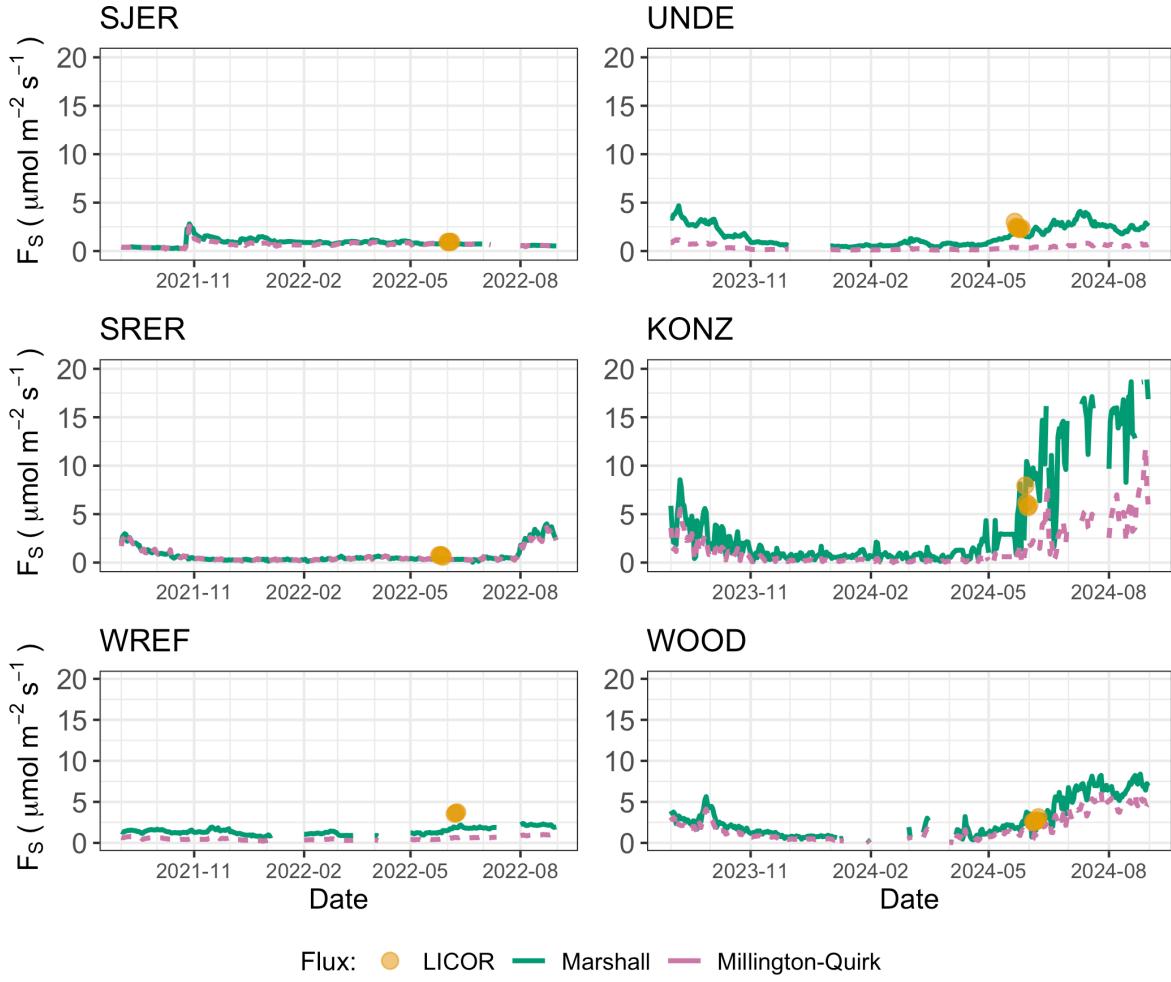


Figure 5: Timeseries of both daily-averaged field F_S (yellow circles) and daily ensemble averaged soil fluxes (average of F_{000} , F_{101} , F_{011} , F_{110} , Section 4.2.3) by the `neonSoilFlux` R package, separated by the diffusivity model used (green or purple lines, Millington-Quirk or Marshall, Section 4.2.2).

distribution of the number of different gap-filled measurements used to compute a half-hourly flux. The largest cause of measurements needing to be gap-filled was missing or flagged soil moisture data. Calculating fluxes for WOOD and SJER required using the largest proportion of gap-filled measurements, due to substantially large fractions of flagged or missing SWC and T_S data.

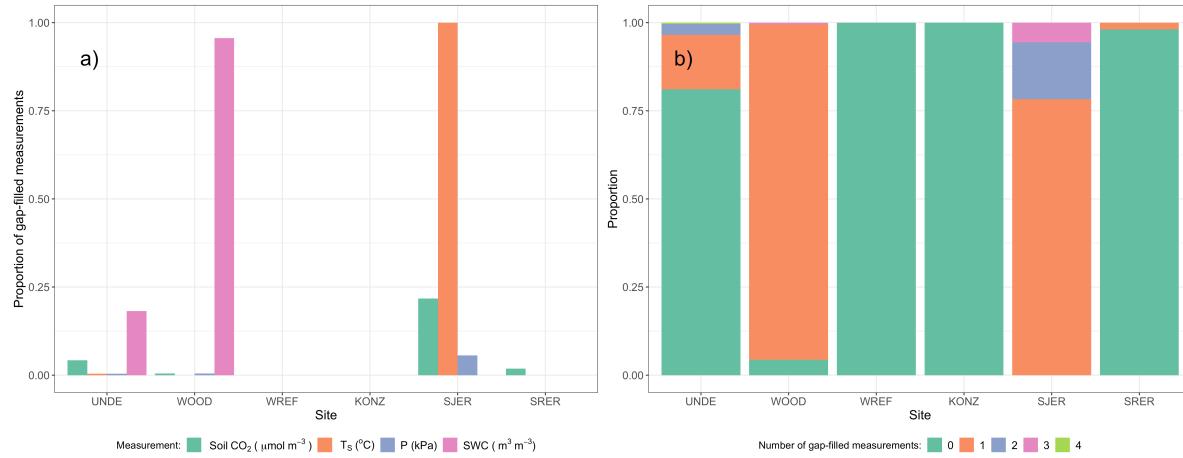


Figure 6: Panel a) Proportion of input gap-filled environmental measurements used to generate F_S from the `neonSoilFlux` package, by study site. Panel b) distribution of the usage of gap-filled measurements at each site.

326 5.4 Assessing the signal to noise ratio (SNR) and evaluating estimated 327 uncertainties

The computed signal to noise ratio (SNR) and the proportion of measured field fluxes within the modeled uncertainty for a given flux computation method F_{ijk} suggest that there was substantial variability in the agreement between the gradient method and field-measured observations (Figure 7, Section 4.3). Here, values of SNR greater than unity indicate lower reported uncertainty, as propagated by quadrature due to a relatively higher precision of measured input variables (CO_2 , T_S , SWC, or P).

334 The sensitivity to an uncertainty reduction factor (ϵ , bottom panels in Figure 7) demonstrates
 335 how concordance between measured and modeled fluxes would be affected if environmental
 336 measurement uncertainty σ_{ijk} were to decrease. As ϵ increases from left to right in each figure,
 337 the possible range of values for each predicted flux value decreases and the proportion of
 338 measured fluxes that fall within that range also decreases.

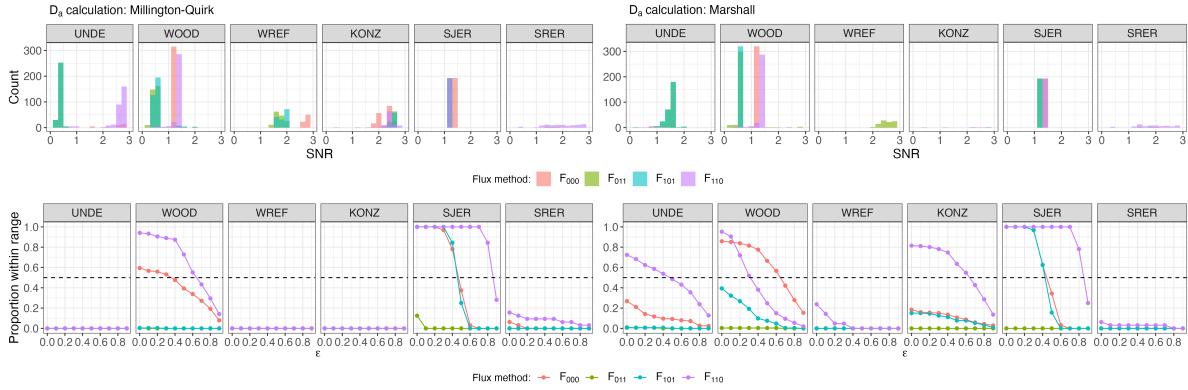


Figure 7: Top panels: distribution of SNR values across each of the different sites for modeled effluxes from the `neonSoilFlux` package, depending on the diffusivity calculation used (Millington-Quirk or Marshall, Section 4.2.2). Bottom panels: Proportion of measured F_S within the modeled range of a flux computation method F_{ijk} given an uncertainty reduction factor ϵ , or $|F_S - F_{ijk}| < (1 - \epsilon)\sigma_{ijk}$.

339 5.5 Effects of method choice on diffusivity estimates

340 We assessed the distribution of D_a (from both the Marshall and Millington-Quirk methods)
 341 at each study site, and also computed a *post hoc* estimate of D_a using field surface flux
 342 measurements (Section 4.2.2). For the field-estimated measurements we omitted negative
 343 values of D_a , as that indicates the CO₂ gradient decreases with soil depth (thereby violating
 344 assumptions of the flux-gradient method, which is our focus here). In four of six field sites,
 345 the *post hoc* estimate fell roughly between the two diffusion estimation methods; however this
 346 was less the case in the two driest sites, SJER and SRER (Table 1), where the field estimate
 347 of diffusivity was either lower or higher than both of the other methods (Figure 8).

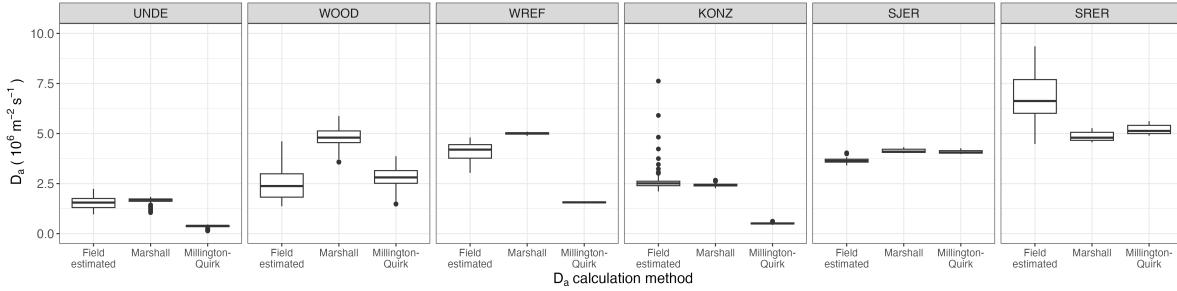


Figure 8: Distribution of diffusivity (D_a) at each study site. Values of D_a were provided by the `neonSoilFlux` package, computed from the Millington-Quirk or Marshall models (Section 4.2.2). A post-hoc estimate of diffusivity (labeled as “Field estimated”) was computed through the field measured flux (Figure 4), divided by the CO_2 gradient from the measurement levels closest to the soil surface, as reported by NEON. We only used F_S measured by the LICOR 6800 at all sites to standardize comparisons.

348 6 Discussion

349 This study presents a unified data science workflow to efficiently process automated measure-
 350 ments of belowground soil CO_2 concentrations, soil water content, and soil temperature to
 351 infer estimates of soil surface CO_2 effluxes through application of Fick’s Law (Equation 4).
 352 Our core goals in this study were: (1) to generate estimates of soil flux from continuous soil
 353 sensor data at terrestrial NEON sites using the flux-gradient method and then (2) to compare
 354 those estimates to field-measured fluxes based on the closed chamber approach at six NEON
 355 focal sites. We discuss our progress toward these core goals through (1) an overall evaluation
 356 of the flux-gradient approach (and uncertainty calculation) and (2) site-specific evaluation of
 357 differences in estimated vs measured fluxes.

358 6.1 General evaluation of flux-gradient approach

359 Key assumptions of the flux-gradient approach are that CO_2 concentrations increase through-
 360 out the soil profile such that the highest concentrations are observed in the deepest layers.

361 Additionally, field flux measurements should correlate with F_{000} because they represent sur-
362 face fluxes. Periods where this gradient condition are not met generally are connected to
363 processes that occur during soil wetting events, where more shallow soil layers produce higher
364 concentrations of CO₂ due to microbial respiration pulses following rewetting. This effect is
365 likely to be largest at sites with rich organic soils (e.g. KONZ). Based on this reasoning, in
366 these types of situations we would *a priori* expect $F_{011} \leq F_{101} \leq F_{110} \leq F_{000}$ because the
367 previous flux estimates rely primarily on CO₂ concentrations at deeper depths, and could miss
368 high concentrations of CO₂ produced in shallower layers.

369 When modeling soil respiration, typically a non-linear response function that also considers soil
370 type is used (Bouma & Bryla, 2000; Yan et al., 2016, 2018). For the `neonSoilFlux` package,
371 our characterization of soil type is connected to the measurement of bulk density, which was
372 characterized at each NEON site. This bulk density estimate is based on replicate samples
373 collected from the site megapit at a subset of soil horizons, with an estimated uncertainty of
374 ±5% (National Ecological Observatory Network (NEON), 2024c). Coarse fragment estimates
375 also have very large uncertainties, but because the volume fraction tends to be low in surface
376 soils it probably wouldn't contribute much additional flux uncertainty.

377 Our results suggest that the most important way to improve reliability of the flux estimate is
378 to reduce the usage of gap-filled data. The current approach to gap filling in `neonSoilFlux`
379 uses monthly mean data to gap fill—this approach decreases the ability of the estimate to
380 be responsive to short turn pulses that occur with rapid weather shifts. Four sites (KONZ,
381 SRER, WREF, and UNDE) had more than 75% of half-hourly periods with no-gap filled
382 measurements. Two sites (SJER and WOOD) had more than 75% of half-hourly intervals
383 with just one gap-filled measurement. While we did not need to use gap-filled measurements
384 to compute the flux at WREF, field data collection occurred following a severe rainstorm, with
385 soils at the beginning of the sampling week near their water holding capacity. We recommend

386 that whenever possible, knowledge of local field conditions should influence analysis decisions
387 in addition to any QA filtering protocols in the `neonSoilFlux` package.

388 We recognize that this gap-filling approach may lead to gap-filled values that are quite different
389 from the actual values, such as an underestimate of soil moisture following rain events. Further
390 extensions of the gap filling method could use more sophisticated gap-filling routines, similar to
391 what is used for net ecosystem carbon exchange (Falge et al., 2001; Liu et al., 2023; Mariethoz
392 et al., 2015; Moffat et al., 2007; Zhang et al., 2023). The current gap-filling routine provides
393 a consistent approach that can be applied to each data stream, but further work may explore
394 alternative gap-filling approaches.

395 **6.2 Evaluation of flux-gradient approach at each site**

396 Derived results from the `neonSoilFlux` package have patterns that are broadly consistent
397 with those directly measured in the field (Figure 4 and Figure 5). One advantage of the
398 `neonSoilFlux` package is its ability to calculate fluxes across different soil depths (Figure 3),
399 which allows for additional site-specific customization. We believe the package can provide
400 a useful baseline estimate of soil fluxes that can always be complemented through additional
401 field measurements.

402 The six locations studied provide a range of case studies that suggest different considerations
403 may apply to different sites when applying the flux-gradient method. For example, the Santa
404 Rita Experimental Range (SRER) is a desert site characterized by sandy soil, which also was
405 the location of the highest field soil temperatures that we observed (?@tbl-licor-summary).
406 At SRER the flux across the top two layers (F_{110}) produced a pattern of soil flux most con-
407 sistent with the observed field data. The remaining methods F_{101} , F_{011} , or F_{000} are derived
408 from information taken from the deepest layer, which seems to have been decoupled from the

409 surface layers both in terms of temperature and CO₂ concentration. This may be a general
410 circumstance where there are large diurnal temperature extremes that rapidly change during
411 the course of a day and overnight, leading to lags in the timing of when temperature increases
412 propagate down to deeper soil layers.

413 Immediately prior to our visit to Konza Prairie (KONZ), that site that experienced a significant
414 rain event that led to wet soils that gradually dried out over the course of our time there.
415 This pulse of precipitation increased the soil CO₂ concentration at the top layer above the
416 concentrations in lower layers, leading to negative estimated flux values at the start of the
417 experiment. In this case it was only when the soil began to return to a baseline level that the
418 assumptions of the flux-gradient method were again met.

419 Thus, when considering systematic deployment of this method across a measurement network,
420 there are a number of independent challenges that require careful consideration. There are clear
421 tradeoffs between (1) accuracy of modeled fluxes (defined here as closeness to field-measured
422 F_S and the uncertainty reduction factor ϵ), (2) precision (defined by the SNR), and (3) the
423 choice of the diffusivity model (Section 4.2.2) or flux computation method (Section 4.2.3)
424 used (Figure 7). There was no predictable pattern in SNR for either the flux computation
425 method or diffusivity calculation, indicating that output uncertainty is driven primarily by
426 input measurement uncertainty (T_S , P , SWC, or CO₂). Across the different flux computation
427 methods, the proportion of measured fluxes where $|F_S - F_{ijk}| < (1 - \epsilon)\sigma_{ijk}$ decreased as
428 ϵ increased, except where field F_S was already outside of the modeled range (i.e. UNDE
429 and WREF). The method F_{110} (where soil flux was computed from the top two soil layers)
430 was the least sensitive to the uncertainty reduction factor (ϵ). This lack of sensitivity could
431 represent that a surface chamber-based measurement method (e.g. with a LI-COR instrument)
432 measures the flux up out of the surface layer and thus is most closely related to assumptions
433 and measurements inherent in the F_{110} method.

434 Finally, comparing the effects of different diffusivity estimation methods on the match between
435 modeled and measured fluxes (Figure 5) highlights the sensitivity of F_{ijk} to diffusivity. The
436 comparison between diffusivity estimates compared to field estimated diffusivity (Figure 8)
437 demonstrates that site parameters can dictate which measure of diffusivity is most likely to
438 be accurate in a given environmental context. Site-specific differences a largely a reflection of
439 differences in soil moisture across the sites (Table 1), as not all diffusivity estimation methods
440 incorporate soil moisture equivalently. While we here have compares two approaches to cal-
441 culate diffusivity (the Millington-Quirk and Marshall models), it may be valuable to evaluate
442 other diffusivity models (e.g. the Moldrup model Moldrup et al. (1999)) as well. Ultimately the
443 choice of a particular diffusivity model could be determined based on knowledge of site-specific
444 evaluations or a set of these models could be used to generate a model ensemble average as a
445 means to trade precision for a more general approach.

446 6.3 Recommendations for future method development

447 The `neonSoilFlux` package provides three different approaches to estimate soil flux using the
448 gradient method. We believe these approaches enable the software to be used across a range of
449 site-specific assumptions (Maier & Schack-Kirchner, 2014). We note, however, that this choice
450 can have a determinative approach on the calculated values. Ensemble averaging approaches
451 (Elshall et al., 2018; Raftery et al., 2005) may be one way to address this problem if the goal is
452 to calculate fluxes using the same method at a diverse range of different sites. Two other ideas
453 would be to apply machine learning algorithms (e.g. random trees) to generate a single flux
454 estimate across diverse sites, or using co-located estimates of net ecosystem carbon exchange
455 from eddy-flux towers to further constrain results or to assess soil flux results for plausibility.

456 These challenges notwithstanding, the method used here and made available in the
457 `neonSoilFlux` R package has the potential to produce nearly continuous estimates of flux

458 across all terrestrial NEON sites. These estimates are a significant improvement on available
459 approaches to constrain the portion of ecosystem respiration attributable to the soil. This,
460 in turn, also aids in our ability to understand the soil contribution to the net ecosystem flux
461 measured at these sites using the co-located eddy flux towers.

462 7 Conclusions

463 We have here presented an R package `neonSoilFlux` for the estimation of soil CO₂ fluxes from
464 continuous buried soil sensor measurements across terrestrial National Ecological Observatory
465 Network sites. We compared the predicted fluxes to those measured directly using a field-based
466 closed chamber approach. We find that the flux gradient method, while broadly effective at
467 producing estimates of flux comparable to those measured in the field using a chamber-based
468 technique, is quite sensitive to a number of issues, including most prominently: missing data
469 (and thus gap-filling of input measurement datasets) the selection of soil depths used to best
470 calculate the gradient (which may vary between sites), and finally the choice of method used
471 for estimating soil diffusivity. Despite these challenges, the broad geographic scale and high
472 temporal resolution of the NEON data make a compelling case for continued efforts to refine
473 this approach to help us understand how soils across diverse ecosystems are responding to a
474 changing climate.

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