

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
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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
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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.

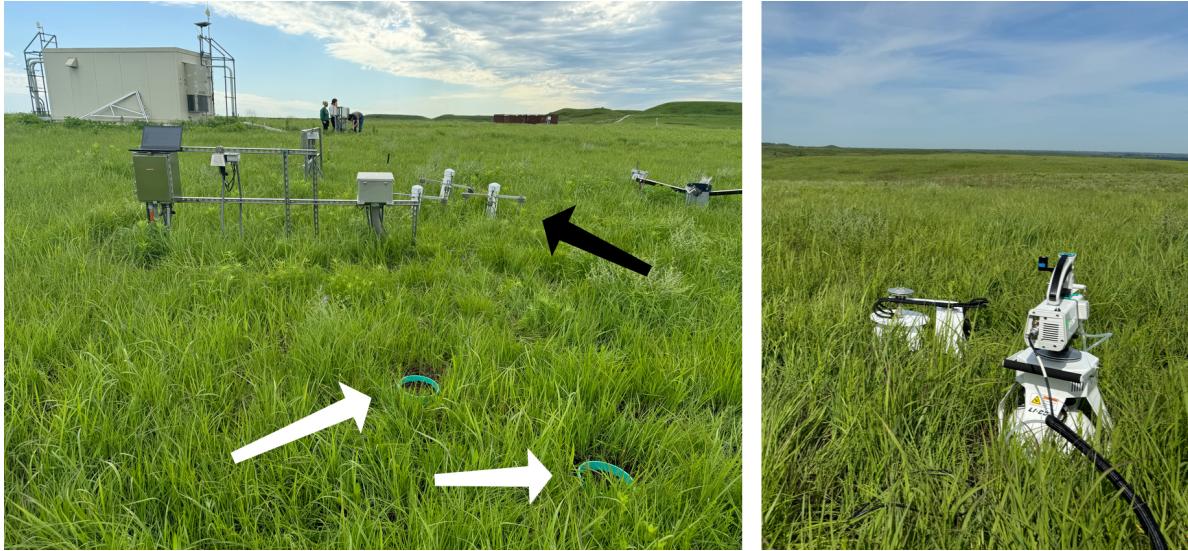


Figure 1: Spatial layout of field sampling using a closed-dynamic chamber setup at a representative NEON site (KONZ). Left image shows collars (white arrows) and permanent soil sensor installation (black arrow) and right image shows the LI-6800 (foreground) and LI-8200-104 (background) instruments placed 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
Wind River Experimental Forest (WREF)	45.82049, -	Evergreen forest	9.2°C	15.3°	2225 mm	27.2%	07 June 2022	001
Chase Lake National Wildlife Refuge (WOOD)	121.95191	Restored prairie	4.9°C	14.9°	495 mm	14.9%	03 June 2024 - 09	001
Konza Prairie Biological Station (KONZ)	47.1282, -	Tallgrass prairie	12.4°C	23.4°	870 mm	23.4%	29 May 2024 - 01	001
	99.241334	grassland					June 2024	
	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).

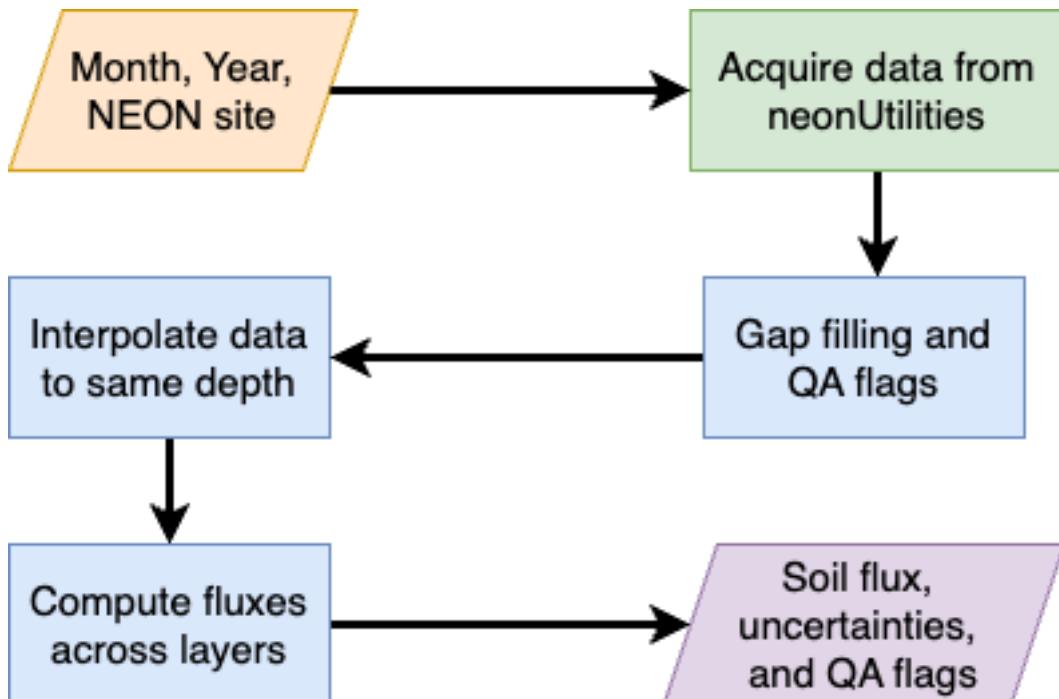


Figure 2: Diagram of `neonSoilFlux` R package. For a given month, year, and NEON site (orange parallelogram), the package acquires all relevant data to compute F_S using the `neonUtilities` R package (green rectangle). Data are gap-filled according to reported QA flags and interpolated to the same measurement 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.

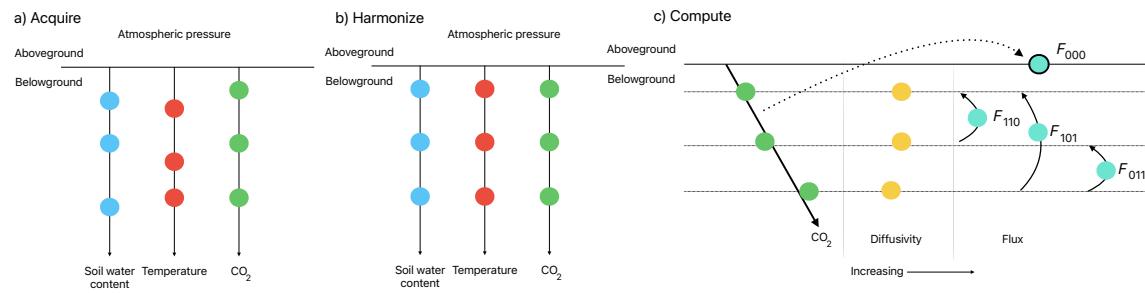


Figure 3: Model diagram for data workflow for the `neonSoilFlux` R package. a) Acquire: Data are obtained from given NEON location and horizontal sensor location, which includes soil water content, soil temperature, CO₂ concentration, and atmospheric pressure. All data are screened for quality assurance; 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 The timeseries of the measured fluxes from the LI-COR 6800 and 870/8250 were compared
 288 to modeled soil fluxes from the `neonSoilFlux` R package (Figure 4). We also assessed year-
 289 long estimated flux time series and compared those field measurements for each measurement
 290 site (Figure 5). Results are reported in local time. Where applicable, sites are displayed
 291 by increasing soil temperature (Table 1). Positive values of the flux indicate that there is
 292 a flux moving towards the surface. For ease of clarity the fluxes at F_{111} and F_{000} are only
 293 shown in the top row (surface), followed by the fluxes at individual separate layers (F_{100} , F_{010} ,
 294 F_{001}). Overall, with the exception of WREF and SRER (discussed later) the computed fluxes
 295 determined using a variety of plausible methods spanned the measured field fluxes.

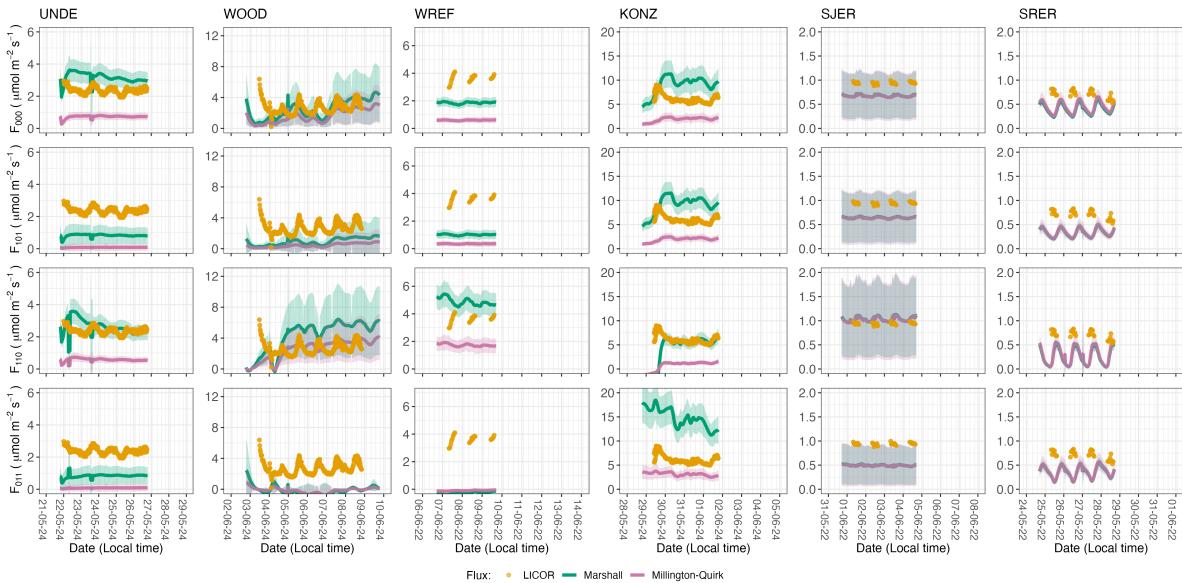


Figure 4: Timeseries of both measured F_S (yellow circles) and modeled soil fluxes (green or purple lines) by the `neonSoilFlux` R package. Fluxes from the `neonSoilFlux` R package are separated by the diffusivity model used (Millington-Quirk or Marshall, Section 4.2.2). Vertical axis labels in the first 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.

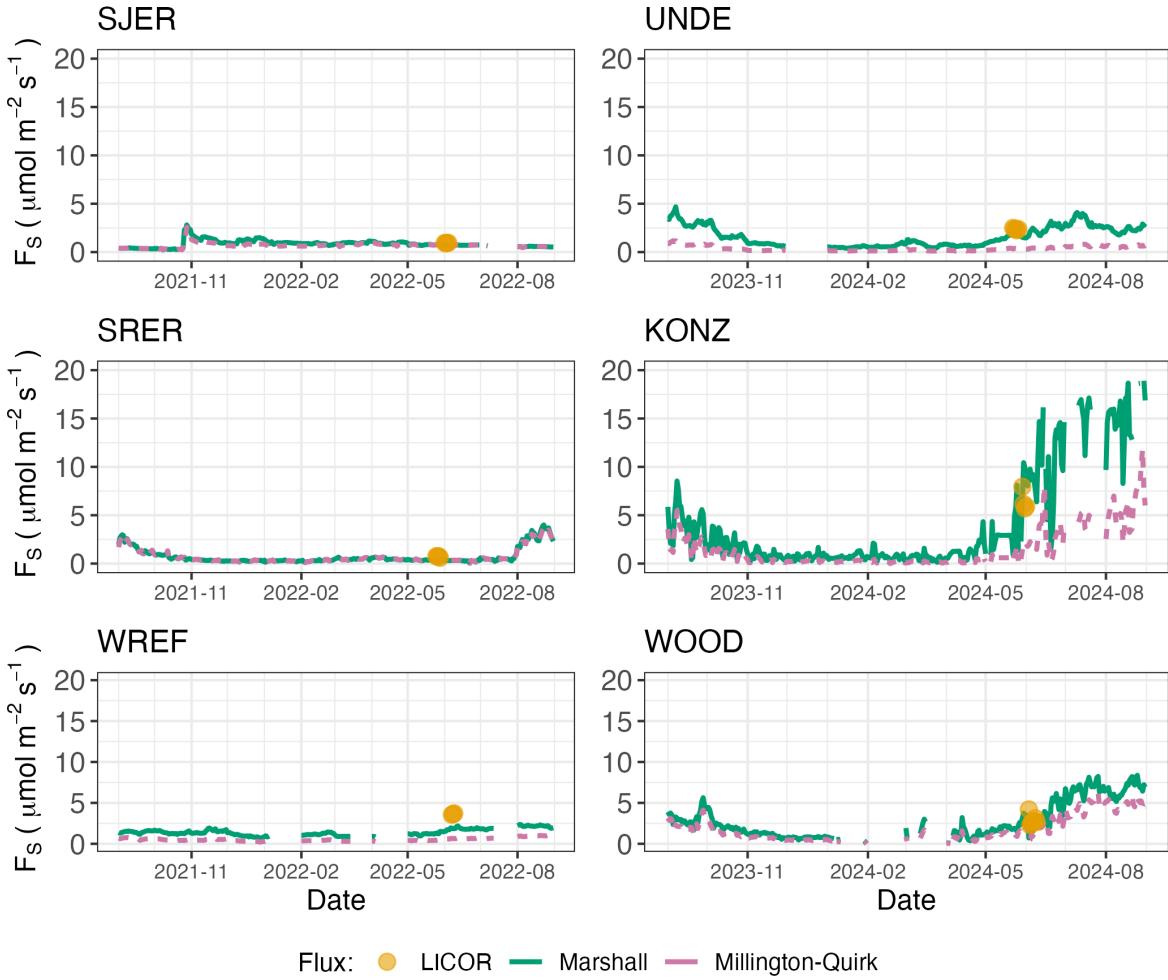


Figure 5: Timeseries of both daily-averaged field F_S (yellow circles) and daily ensemble averaged soil fluxes (green or purple lines) by the `neonSoilFlux` R package, separated by the diffusivity model used (Millington-Quirk or Marshall, Section 4.2.2). The time-series of modeled fluxes are a daily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

296 Table 2 compares statistics of the modeled soil fluxes to field F_S at each site. As `neonSoilFlux`
 297 models half-hourly fluxes, we considered all measured fluxes over the duration of the half-hourly
 298 interval when computing the normalized root mean square error (NRMSE), R^2 , at each of the
 299 flux methods (F_{000} , F_{110} , F_{011} , F_{101}) for the diffusivity models studied (Millington-Quirk or
 300 Marshall).

301 For a given half-hourly time period, the `neonSoilFlux` packages assigns a QA flag for a mea-
 302 surement if more one values across all measurement depths uses gap-filled data (Section 4.2.1).
 303 Panel a of Figure 6 reports the distribution for all input environmental measurements at each
 304 site when field measurements were made. Soil fluxes are computed from 4 different types of
 305 input measurements (T_S , SWC , P , and CO_2), any of which could have a QA flag in a half-
 306 hourly interval. Panel b of Figure 6 displays at each site the distribution of the number of
 307 different gap-filled measurements used to compute a half-hourly flux. The largest contribution
 308 to gap-filled measurements was soil water. SJER and WOOD utilized the largest number of
 309 gap-filled measurements, which were primarily SWC and T_S .

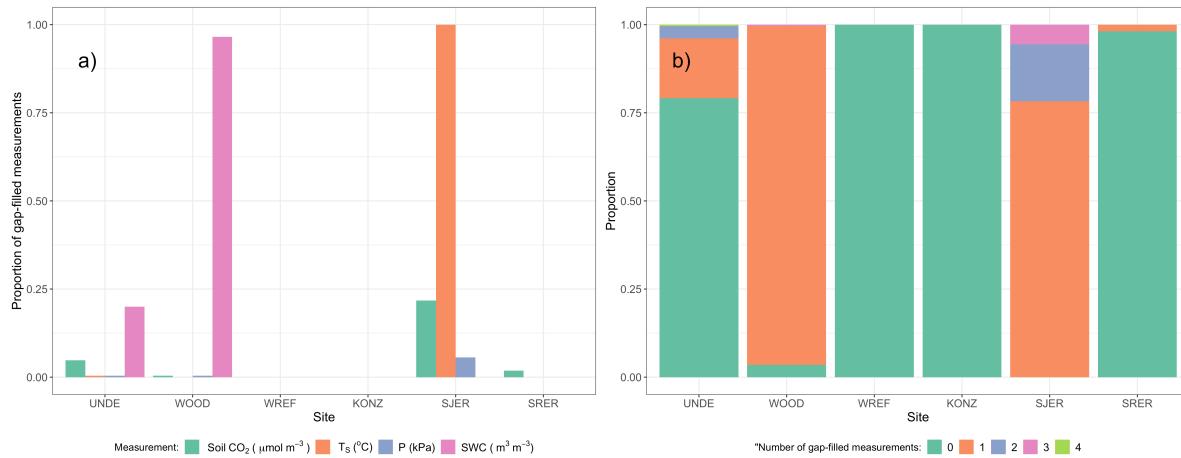


Figure 6: Panel a) Proportion of input gap-filled environmental measurements used to generate F_S from the `neonSoilFlux` package, by study site. Panel b) distribution of the usage of gap-filled measurements at each site.

310 Figure 7 reports both the computed SNR and the proportion of measured field fluxes within the

Table 2

	Millington-Quirk		Marshall	
	NRMSE	R2	NRMSE	R2
KONZ				
F_{110}	0.87	0.41	0.63	0.41
F_{101}	0.69	0.22	0.60	0.15
F_{011}	0.52	0.20	1.35	0.25
F_{000}	0.70	0.23	0.58	0.14
SJER				
F_{110}	0.13	0.17	0.14	0.19
F_{101}	0.32	0.21	0.31	0.24
F_{011}	0.49	0.02	0.48	0.03
F_{000}	0.29	0.18	0.28	0.19
SRER				
F_{110}	0.56	0.00	0.59	0.00
F_{101}	0.66	0.53	0.67	0.52
F_{011}	0.69	0.49	0.70	0.49
F_{000}	0.58	0.51	0.61	0.51
UNDE				
F_{110}	0.76	0.10	0.25	0.02
F_{101}	0.97	0.28	0.66	0.21
F_{011}	0.97	0.15	0.66	0.06
F_{000}	0.70	0.30	0.38	0.05
WOOD				
F_{110}	0.44	0.03	0.93	0.02
F_{101}	0.89	0.07	0.74	0.05
F_{011}	1.12	0.02	1.22	0.01
F_{000}	0.56	0.06	0.46	0.05
WREF				
F_{110}	0.53	0.78	0.35	0.75
F_{101}	0.91	0.24	0.73	0.35
F_{011}	1.03	0.37	1.07	0.37
F_{000}	0.84	0.00	0.49	0.05

modeled uncertainty for a given flux computation method F_{ijk} (Section 4.3). Here, values of SNR greater than unity indicates a reported uncertainty is smaller, propogated by quadrature from a relatively higher precision from measured input variables (CO_2 , T_S , SWC , or P). The sensitivity to the uncertainty reduction factor (ϵ , bottom panels in Figure 7) demonstrates how accuracy could be improved if modeled uncertainty σ_{ijk} decreases.

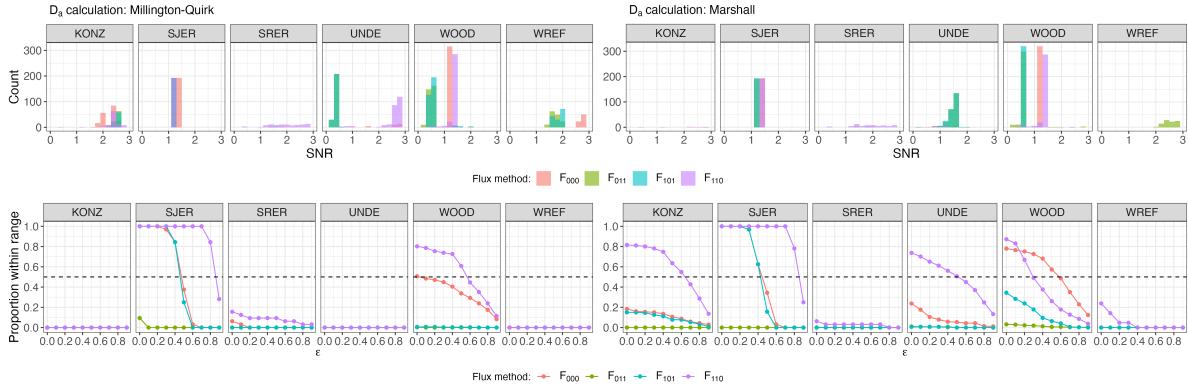


Figure 7: Top panels: distribution of SNR values across each of the different sites for modeled effluxes from the `neonSoilFlux` package, depending on the diffusivity calculation used (Millington-Quirk or Marshall, Section 4.2.2). Bottom panels: Proportion of measured F_S within the modeled range of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

Figure 8 reports the distribution of D_a (from both the Marshall and Millington-Quirk methods, Section 4.2.2) at each study site, and the *post hoc* computation of D_a (Section 4.2.2). Over the course of a half-hourly interval the same CO_2 gradient (from `neonSoilFlux`) was used for the different LICOR measured fluxes. We only used F_S measured by the LICOR 6800 at all sites to standardize comparisons. For the field-estimated measurements we omitted negative values of D_a , as that indicates the CO_2 gradient decreases with soil depth (thereby violating assumptions of the flux-gradient method).

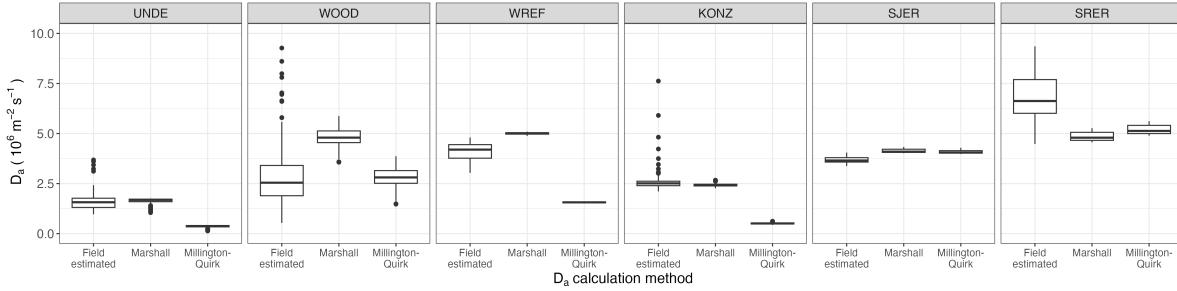


Figure 8: Distribution of diffusivity (D_a) at each study site. Values of D_a were provided by the `neonSoilFlux` package, computed from the Millington-Quirk or Marshall models (Section 4.2.2). A post-hoc estimate of diffusivity (labeled as “Field estimated”) was computed through the field measured flux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

6 Discussion

This study presents a unified data science workflow to efficiently process automated measurements of belowground soil CO_2 concentrations, water, and temperature to infer estimates of soil surface CO_2 effluxes through application of Fick’s Law (Equation 4). 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 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.

6.1 General evaluation of flux-gradient approach

Key assumptions of the flux-gradient approach are that CO_2 concentrations increase throughout the soil profile. Periods where this gradient condition are not met generally are connected

336 to biophysical processes such soil wetting events (e.g. KONZ), which have the effect of reduc-
337 ing the soil respiration or efflux due to a temporary reduction in diffusivity. When modeling
338 soil respiration, typically a non-linear response function that also considers soil type is used
339 (Bouma & Bryla, 2000; Yan et al., 2016, 2018). For the `neonSoilFlux` package, soil type is
340 connected to the bulk density, which was characterized at each NEON site based on replicate
341 samples collected from the site megapit at a subset of soil horizons, with an estimated un-
342 certainty of $\pm 5\%$ (see NEON User Guide to Soil physical and chemical properties, Megapit
343 (DP1.00096.001)). Coarse fragment estimates also have very large uncertainties, but because
344 the volume fraction tends to be low in surface soils it probably wouldn't contribute much
345 additional flux uncertainty.

346 The largest source of uncertainty to improve reliability of the flux estimate is to prevent the
347 usage of gap-filled data. Three sites (KONZ, SRER, and KONZ) had more than 75% of half-
348 hourly periods with no-gap filled measurements. Two sites (SJER and WOOD) had more
349 than 75% of half-hourly intervals with just one gap-filled measurement. While WREF re-
350 ported no gap-filled measurements, field data collection occurred following a once-in-a century
351 rainstorm with soils observed at their water holding capacity. We recommend that whenever
352 available, local field knowledge is supplementary to any QA filtering protocol of fluxes from
353 the `neonSoilFlux` package.

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

361 Based on this approach, we would *a priori* expect $F_{011} \leq F_{101} \leq F_{110} \leq F_{000}$ because the
362 previous flux estimates ones correspond to deeper depths which will could miss CO₂ produced
363 in shallower layers. Additionally, field flux measurements should correlate with F_{000} because
364 they represent surface fluxes.

365 **6.2 Evaluation of flux-gradient approach at each site**

366 Derived results from the `neonSoilFlux` package have patterns that are consistent, and com-
367 parable, to those directly measured to the field (Figure 4 and Figure 5). The advantage to
368 the `neonSoilFlux` package is the calculation of fluxes across different measurement depths, al-
369 lowing for additional site-specific customization. Here application of the flux-gradient method
370 provides a baseline estimate of soil fluxes that could be complemented through additional field
371 measurements (e.g. LICOR).

372 The six sites studied provide separate case studies for considerations when applying the flux-
373 gradient method to evaluate resulting uncertainties and fluxes For example, SRER is charac-
374 terized by sandy soil, which also led to the highest observed field soil temperatures. At SRER
375 the flux across the top two layers (F_{110}) produced a pattern of soil flux consistent with the ob-
376 served field data. The remaining methods F_{101} , F_{011} , or F_{000} are derived from information at
377 the deeper layer, which is decoupled both in terms of temperature and CO₂ concentration.

378 In addition, KONZ is a site that experienced a significant rain event prior to sampling with
379 eventual drying out over the course of the experiment. In this case we observed storage of soil
380 water which increased the soil CO₂ at the top layer, leading to negative values of flux at the
381 start of the experiment, with the fluxes drying out afterwards. In this case only when the soil
382 dried out (or returned to a baseline level), that the fluxes at the provided layer would work
383 out in this case.

When considering systematic deployment of this method across a measurement network, we faced a number of independent challenges for consideration. Figure 7 illustrates tradeoffs between (1) accuracy for modeled fluxes (defined here as closeness to field-measured F_S and the uncertainty reduction factor ϵ), (2) precision (defined by the SNR), and (3) the choice of the diffusivity model (Section 4.2.2) or flux computation method (Section 4.2.3). There was no predictable pattern in SNR for either the flux computation method or diffusivity calculation, indicating that output uncertainty is driven primarily by input measurement uncertainty (T_S , P , SWC, or CO₂). Across the different flux computation methods, the proportion of measured fluxes where $|F_S - F_{ijk}| < (1-\epsilon)\sigma_{ijk}$ decreased as ϵ increased, except where field F_S was already outside of the modeled range (i.e. UNDE and WREF). The method F_{110} (where soil flux was computed from the top two soil layers) was the least sensitive to the uncertainty reduction factor (ϵ). This lack of sensitivity could represent that the LICOR samples from the top surface layer, and is most closely related to assumptions of the F_{110} method.

Comparing diffusivity methods to field estimated diffusivity (Figure 8) highlights the sensitivity of F_{ijk} to diffusivity. Site-specific differences reflect the soil moisture availability across the site (Table 1), and also reflect the model variation in Figure 4. While here we compare two approaches to calculated diffusivity (Millington-Quirk or Marshall model), other diffusivity models (e.g. the Moldrup model Moldrup et al. (1999)) could be evaluated. Ultimately the choice of a particular diffusivity model could be determined through site-specific evaluated or a source of model output uncertainty (e.g. as a model ensemble average).

6.3 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

408 method having a determinative approach on reported values. Reported results could further
409 be distilled down using ensemble averaging approaches (Elshall et al., 2018; Raftery
410 et al., 2005).

411 These challenges notwithstanding, the method used here and made available in the
412 `neonSoilFlux` R package has the potential to produce nearly continuous estimates of flux
413 across all terrestrial NEON sites. These estimates are a significant improvement on available
414 approaches to constrain the portion of ecosystem respiration attributable to the soil. This, in
415 turn, aids in our ability to understand the components of net ecosystem flux assessed at these
416 sites using the co-located eddy flux towers.

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

422 7 Conclusions

423 We have here presented an R package `neonSoilFlux` for the estimation of soil CO₂ fluxes from
424 continuous buried soil sensor measurements across terrestrial National Ecological Observatory
425 Network sites. We compared the predicted fluxes to those measured directly using a field-based
426 closed chamber approach. We find that...

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