

¹ **neonSoilFlux: An R Package for Continuous
2 Sensor-Based Estimation of Soil CO₂ Fluxes**

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¹³ **Acknowledgments**

¹⁴ John Zobitz acknowledges Kathleen O'Rourke for code development. Naupaka Zimmerman
¹⁵ thanks technical staff at USF for support with field gear assembly and shipping. We thank the
¹⁶ NEON field staff and assignable assets teams for facilitating each of the six NEON site visits.

¹⁷ We are grateful to LI-COR technical staff for helpful discussions about optimal soil chamber
¹⁸ sampling methods. This work was supported by NSF DEB grant #2017829 awarded to John
¹⁹ Zobitz, and NSF DEB grant #2017860 awarded to Naupaka Zimmerman. This material is
²⁰ based in part upon work supported by the National Ecological Observatory Network (NEON),
²¹ a program sponsored by the U.S. National Science Foundation (NSF) and operated under
²² cooperative agreement by Battelle. We also thank the reviewers and subject editor for their
²³ constructive feedback.

²⁴ **Conflict of Interest Statements**

²⁵ None of the authors have a financial, personal, or professional conflict of interest related to this
²⁶ work.

²⁷ **Author Contributions**

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³⁹ Project Administration: John Zobitz, Naupaka Zimmerman; Funding Acquisition: John Zobitz,
⁴⁰ Naupaka Zimmerman.

⁴¹ **Data Availability**

⁴² Data available via <https://doi.org/10.5281/zenodo.17516319> (Zobitz & Zimmerman, 2025).
⁴³ Field-collected data, `neonSoilFlux` calculated outputs, and manuscript-generating code are
⁴⁴ provided within this repository.

45 **1 Abstract**

- 46 1. Accurate quantification of soil carbon fluxes is essential to reduce uncertainty in estimates
47 of the terrestrial carbon sink. However, these fluxes vary over time and across ecosystem
48 types and so it can be difficult to estimate them accurately across large scales. The flux
49 gradient method estimates soil carbon fluxes using co-located measurements of soil CO₂
50 concentration, soil temperature, soil moisture, and other soil properties. The National
51 Ecological Observatory Network (NEON) provides such data across 20 ecoclimatic domains
52 spanning the continental U.S., Puerto Rico, Alaska, and Hawai‘i.
- 53 2. We present an R software package (`neonSoilFlux`) that acquires soil environmental data
54 to compute half-hourly soil carbon fluxes for each soil replicate plot at a given terrestrial
55 NEON site. To assess the computed fluxes, we visited six focal NEON sites and measured
56 soil carbon fluxes using a closed-dynamic chamber approach.
- 57 3. Outputs from the `neonSoilFlux` showed agreement with measured fluxes (R^2 between
58 measured and `neonSoilFlux` outputs ranging from 0.04 to 0.81 depending on calculation
59 method used); measured outputs generally fell within the range of calculated uncertainties
60 from the gradient method. Calculated fluxes from `neonSoilFlux` aggregated to the daily
61 scale exhibited expected site-specific seasonal patterns.
- 62 4. While the flux gradient method is broadly effective, its accuracy is highly sensitive
63 to site-specific inputs, including the extent to which gap-filling techniques are used to
64 interpolate missing sensor data and to estimates of soil diffusivity and moisture content.
65 Future refinement and validation of `neonSoilFlux` outputs can contribute to existing
66 databases of soil carbon flux measurements, providing near real-time estimates of a critical
67 component of the terrestrial carbon cycle.

68 **1.1 Keywords**

69 Soil carbon, carbon dioxide, flux gradient, carbon cycle, field validation, soil respiration,
70 ecosystem variability, diffusion

71 **2 Data for peer review**

72 Anonymous field-collected data, `neonSoilFlux` calculated outputs, and manuscript-generating
73 code for peer review are provided as supplemental files. An anonymous link for peer-review
74 is here: <https://doi.org/10.5281/zenodo.16951117>. This will be made publicly available upon
75 publication.

76 **3 Introduction**

77 Soils contain the planet's largest reservoir of terrestrial carbon (Jobbágy & Jackson, 2000). A
78 critical component of this reservoir is soil organic matter, the accumulation of which is influenced
79 by biotic factors such as above-ground plant inputs (Jackson et al., 2017). These inputs in
80 turn are influenced by environmental factors such as growing season length, temperature, and
81 moisture (Desai et al., 2022), which also affect the breakdown of soil organic matter and its
82 return to the atmosphere. Across heterogeneous terrestrial landscapes, the interplay between
83 these biotic and abiotic factors influence the size of the soil contribution to the terrestrial
84 carbon sink (Friedlingstein et al., 2025). However, the heterogeneity of these processes across
85 diverse ecosystems in the context of rapid environmental change leads to large uncertainty
86 about the magnitude of this sink in the future, and thus there remains a pressing need to
87 quantify changes in soil carbon pools and fluxes across scales.

88 Ecological observation networks such as the United States' National Ecological Observatory
89 Network (NEON) and others (e.g. the globally-distributed FLUXNET or the European Inte-
90 grated Carbon Observation System) present a significant advancement in the nearly continuous
91 observation of biogeochemical processes at the continental scale. Notably, at 47 terrestrial
92 sites across the continental United States that span 20 ecoclimatic domains, NEON provides
93 half-hourly measurements of soil CO₂ concentration, temperature, and moisture at different
94 vertical depths. Each of these NEON sites also encompasses measurements of the cumulative
95 sum of all ecosystem carbon fluxes in an airshed using the eddy covariance technique (Baldocchi,
96 2014). Soil observations provided by NEON are on the same timescale and standardized with
97 eddy covariance measurements from FLUXNET. These types of nearly continuous observational
98 data (NEON and FLUXNET) can be used to reconcile differences between model-derived
99 or data-estimated components of ecosystem carbon flux (Jian et al., 2022; Luo et al., 2011;
100 Phillips et al., 2017; J. Shao et al., 2015; P. Shao et al., 2013; Sihi et al., 2016).

101 Estimated or observed soil carbon fluxes are a key metric for understanding change in soil
102 carbon pools over time (Bond-Lamberty et al., 2024). A soil carbon flux to the atmosphere (F_S ,
103 units $\mu\text{mol m}^{-2} \text{s}^{-1}$), represents the aggregate process of transfer of soil CO₂ to the atmosphere
104 from physical and biological processes (e.g. diffusion and respiration). Soil carbon fluxes can
105 be assumed to encompass soil carbon respiration from autotrophic or heterotrophic sources
106 (Davidson et al., 2006) and modeled with a exponential Q_{10} paradigm (Bond-Lamberty et al.,
107 2004; Chen & Tian, 2005; Hamdi et al., 2013).

108 One common method by which F_S is measured in the field is through the use of soil chambers
109 in a closed, well-mixed system (Norman et al., 1997) with headspace trace gas concentrations
110 measured with an infrared gas analyzer (IRGA). F_S can also be estimated from soil CO₂
111 measurements at different depths in the soil using the flux-gradient method (Maier & Schack-
112 Kirchner, 2014). Closed-chamber IRGA measurements, while being the most common method,

113 require either frequent in-person site visits or expensive and fragile automated systems. The
114 potential of the gradient method is that fluxes can be estimated from continuous data recorded
115 by robust solid-state sensors. The flux-gradient method is an approach that uses conservation of
116 mass to calculate flux at a vertical soil depth z at steady state by applying Fick's law of diffusion.
117 A simplifying assumption for the flux-gradient method is that there is no mass transfer in the
118 other spatial dimensions x and y (Maier & Schack-Kirchner, 2014). The diffusivity profile, a
119 key component of this calculation, varies across the soil depth as a function of soil temperature,
120 soil volumetric water content, atmospheric air pressure, and soil bulk density (Millington &
121 Shearer, 1971; Moldrup et al., 1999; Sallam et al., 1984).

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

132 This study describes an R software package, `neonSoilFlux`, that computes a standardized
133 estimate of F_S at all terrestrial NEON sites using the flux-gradient method. Using direct
134 chamber-based field observations of soil carbon dioxide flux from a subset of terrestrial NEON
135 sites spanning six states, we provide a direct validation of F_S from `neonSoilFlux`. While
136 open source R software tools currently exist for processing chamber-based flux measurements
137 (Jurasinski et al., 2022; Pedersen, 2024; Rheault et al., 2024; Wilson et al., 2024; Zhao, 2019),

¹³⁸ to our knowledge this is the first package that incorporates NEON data directly.

¹³⁹ Key objectives of this study are to:

- ¹⁴⁰ 1. Apply the flux-gradient method to estimate soil CO₂ flux from continuous sensor mea-
¹⁴¹ surements across six NEON sites.
- ¹⁴² 2. Benchmark estimated soil carbon fluxes against field measurements (e.g. direct chamber
¹⁴³ measurements of soil flux).
- ¹⁴⁴ 3. Identify sources of error in the flux-gradient approach across diverse sites in order to
¹⁴⁵ guide future work.

¹⁴⁶ 4 Materials and Methods

¹⁴⁷ 4.1 Field methods

¹⁴⁸ 4.1.1 Focal NEON Sites

¹⁴⁹ In order to acquire field data to validate model predictions of flux, we selected six terrestrial
¹⁵⁰ NEON sites for analysis. We conducted roughly week-long field measurement campaigns at
¹⁵¹ these sites, which span a range of environmental gradients and terrestrial domains (Table 1).
¹⁵² SJER, SRER, and WREF were visited during May and June of 2022, and WOOD, KONZ, and
¹⁵³ UNDE during May and June of 2024. Permits or waivers were sought and approved prior to
¹⁵⁴ field work at all six sites. In 2022, research activities were conducted whole or in part on the
¹⁵⁵ Wind River Experimental Forest within the Gifford Pinchot National Forest. No permit was
¹⁵⁶ required for this work. Approval for research at San Joaquin Experimental Range was granted
¹⁵⁷ by Dr. Angela White in May 2022 and for research at Santa Rita Experimental Range by
¹⁵⁸ Dr. Mitch McClaran in May 2022. In 2024, permits were received for work at WOOD (Chase

¹⁵⁹ Lake WMD; permit number 62515-24-020), KONZ (Konza Prairie Biological Station; permit
¹⁶⁰ number 766), and UNDE (University of Notre Dame Environmental Research Center; permit
¹⁶¹ number UNDERC-2024-5).

¹⁶² **4.1.2 Soil collar placement**

¹⁶³ Either one (2022 sampling campaign) or two (2024 sampling campaign) PVC soil collars (20.1
¹⁶⁴ cm inside diameter) were installed in close proximity to the permanent NEON soil sensors at
¹⁶⁵ each site (Figure 1). As instruments in the NEON soil sensor arrays can occasionally break
¹⁶⁶ down or stop working, the specific soil plot where we made measurements was chosen at each
¹⁶⁷ site in consultation with NEON staff to maximize likelihood of quality soil sensor measurements
¹⁶⁸ during the duration of the IRGA measurements. The plot selected at each site (out of the 5 in
¹⁶⁹ each replicate array at each site) are presented in the last column of Table 1. After installation,
¹⁷⁰ collar(s) were left to equilibrate for approximately 24 hours prior to any measurements being
¹⁷¹ taken.

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

¹⁷³ In 2022, we then made measurements of flux on an hourly interval for 8 hours each day.
¹⁷⁴ Measurements were taken from roughly 8 am to 4 pm, with the time interval selected to
¹⁷⁵ capture the majority of the diurnal gradient of soil temperature each day. These measurements
¹⁷⁶ were made using a LI-6800 infrared gas analyzer instrument (LI-COR Environmental, Lincoln,
¹⁷⁷ NE) fitted with a soil chamber attachment (attachment 6800-09). In 2024, we again used the
¹⁷⁸ same LI-6800 instrument, but made half-hourly measurements over an approximately 8 hour
¹⁷⁹ period. In addition, in 2024 we also installed a second collar and used a second instrument, an
¹⁸⁰ LI-870 CO₂ IRGA, connected to an automated robotic chamber (LI-COR chamber 8200-104)

controlled by an LI-8250 multiplexer to make automated measurements. The multiplexer was configured to take half-hourly measurements 24 hours a day for the duration of our sampling bout at each site. Each instrument was paired with a soil temperature and moisture probe (Stevens HydraProbe, Stevens Water, Portland, OR) that was used to make soil temperature and moisture measurements concurrent with the CO₂ flux measurements. Chamber volumes were set by measuring collar offsets at each site. System checks were conducted daily for the LI-6800 and weekly for the LI-8250. Instruments were factory calibrated before each field season.

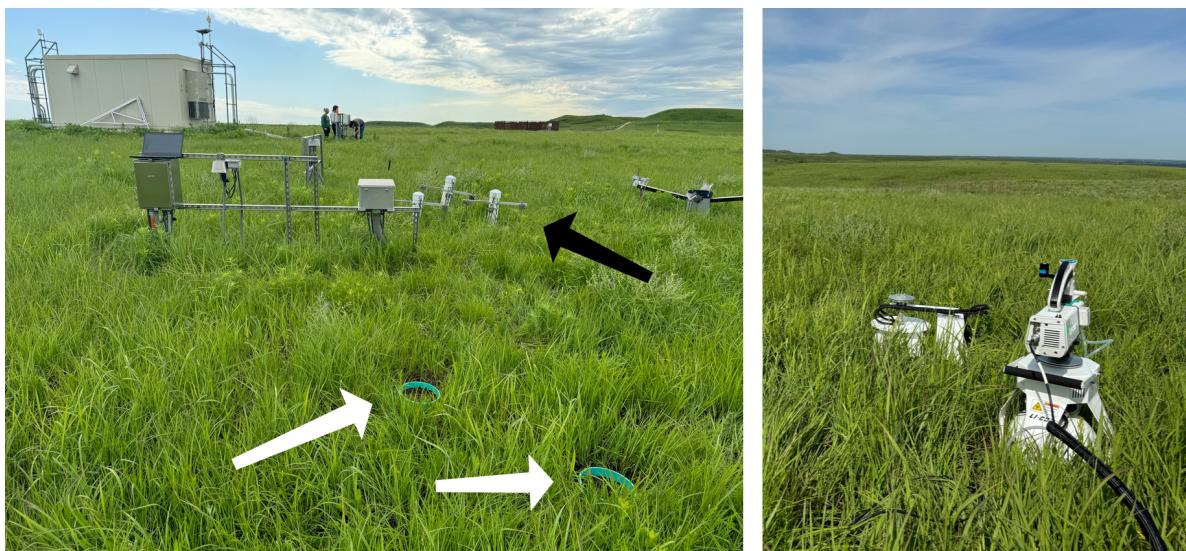


Figure 1: Spatial layout of field sampling using a closed-dynamic chamber setup at a representative NEON site (KONZ). Left image shows collars (white arrows) and permanent soil sensor installation (black arrow) and right image shows the LI-6800 (foreground) and LI-8200-104 (background) instruments placed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

Table 1: Listing of NEON sites studied for field work and analysis. Site refers to NEON site codes: Santa Rita Experimental Range (SRER), San Joaquin Experimental Range (SJER), Wind River Experimental Forest (WREF), Chase Lake National Wildlife Refuge (WOOD), Konza Prairie Biological Station (KONZ), and the University of Notre Dame Environmental Research Center (UNDE). Location is reported in decimal degrees of latitude and longitude. Other abbreviations include Mean Annual Temperature (MAT); \bar{T}_S : average soil temperature during field measurements; \overline{SWC} : average soil water content during field measurements. Dates refer to field measurement dates for each site. Plot refers to the particular location in the soil sensor array (denoted as HOR by NEON) where field measurements were made.

Site	Location	Ecosystem	MAT	\bar{T}_S	MAP	\overline{SWC}	Dates	Plot
SRER	31.91068, -110.83549	Shrubland	19.3 °C	47.6 °C	346 mm	4.0%	May 29– June 1 2022	004
SJER	37.10878, -119.73228	Oak woodland	16.4 °C	41.7 °C	540 mm	1.2%	June 1–4 2022	005
WREF	45.82049, -121.95191	Evergreen forest	9.2 °C	15.3 °C	2225 mm	27.2%	June 7–9 2022	001
WOOD	47.1282, -99.241334	Restored prairie	4.9 °C	14.9 °C	495 mm	14.9%	June 3–9 2024	001
KONZ	39.100774, -96.563075	Tallgrass prairie	12.4 °C	23.4 °C	870 mm	23.4%	May 29– June 1 2024	001
UNDE	46.23391, -89.537254	Deciduous forest	4.3 °C	13.0 °C	802 mm	13.0%	May 22–25 2024	004

189 4.1.4 Post-collection processing of field data

190 We used LI-COR SoilFluxPro software (v 5.3.1) to assess the data after collection and to
 191 inform sampling parameters. We checked appropriateness of dead band and measurement
 192 durations using built-in evaluation tools. Based on this, the deadband period was set for 30-40
 193 seconds, depending on the site, and the measurement duration was 180 seconds with a 30
 194 second pre-purge and a 30 second post-purge at most sites, and a 90 second pre- and post-purge
 195 at sites with higher humidity due to recent precipitation events. We also assessed the R^2 of
 196 linear and exponential model fits to measured CO₂ to verify measurement quality.

197 **4.2 neonSoilFlux R package**

198 We developed an R package called `neonSoilFlux` (Zobitz et al., 2024) to compute half-hourly
199 soil carbon fluxes and uncertainties from NEON data. The objective of the `neonSoilFlux`
200 package is a unified workflow (Figure 2) for soil data acquisition and analysis that supplements
201 the existing `neonUtilities` data acquisition R package (Lunch et al., 2025).

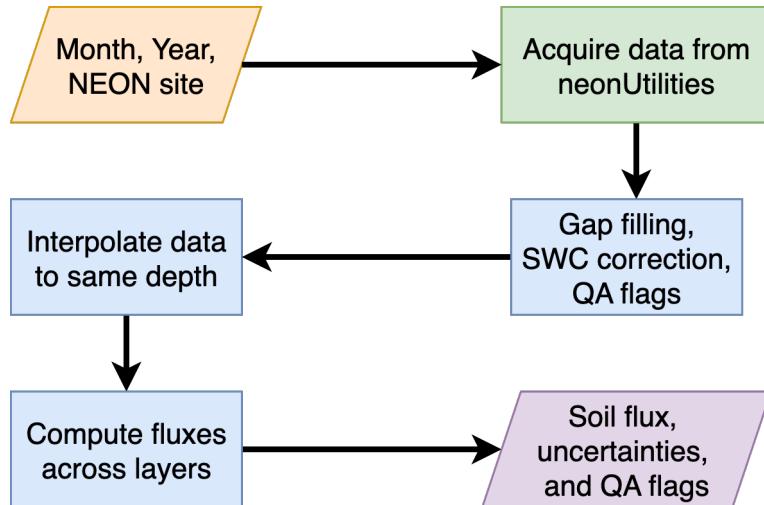


Figure 2: Diagram of `neonSoilFlux` R package. For a given month, year, and NEON site (orange parallelogram), the package acquires all relevant data to compute F_S using the `neonUtilities` R package (green rectangle). Data are gap-filled according to reported QA flags and adjusted for changes in soil water content (SWC) calibration coefficients, then 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).

202 At a given NEON site there are five replicate soil plots, each with measurements of soil
203 CO_2 concentration, soil temperature, and soil moisture at different depths (Figure 3). The
204 `neonSoilFlux` package acquires measured soil CO_2 concentration (NEON, 2024b), soil temper-
205 ature (NEON, 2024d), soil water content (NEON, 2024e), barometric pressure from the nearby
206 tower (NEON, 2024a), and soil properties (e.g. bulk density) (NEON, 2024c) from a range of
207 different NEON data products. The static soil properties were collected by NEON staff from a

208 nearby soil pit during initial site characterization and are assumed to be constant at each site.
 209 A soil flux calculation is computed at each replicate soil plot.

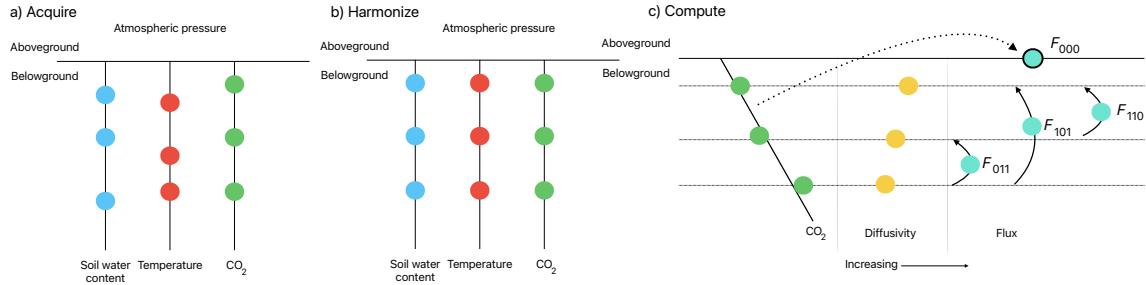


Figure 3: Model diagram of the data workflow for the `neonSoilFlux` R package. a) Acquire: Data are obtained for a given NEON location and horizontal sensor location, which includes soil water content, soil temperature, CO_2 concentration, and atmospheric pressure. All data are screened for quality assurance; if gap-filling of missing data occurs, it is flagged for the user. b) Harmonize: Any belowground data are then harmonized to the same depth as CO_2 concentrations using linear regression. c) Compute: 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 ($i = \text{closest to surface}$, $k = \text{deepest}$). F_{000} represents a flux estimate where the gradient dC/dz is the slope of a linear regression of CO_2 with depth.

210 The workflow to compute a value of F_S with `neonSoilFlux` consists of three primary steps,
 211 illustrated in Figure 3. First, NEON data are acquired for a given site and month via the
 212 `neonUtilities` R package (yellow parallelogram and green rectangle in Figure 2 and Panel a
 213 in Figure 3). Acquired environmental data can be exported to a comma separated value file for
 214 additional analysis. Quality assurance (QA) flags are reported as an indicator variable. Since
 215 the calibration coefficients on the soil water content sensors have changed over time (NEON,
 216 2024e), raw sensor measurements were back-calculated and soil-specific calibrations were applied
 217 following Ayres et al. (2024) to generate a consistent time series at each measurement location.

218 The second step is harmonizing the data to compute soil fluxes across soil layers. This
 219 step consists of three different actions (blue rectangles in Figure 2 and Panel b in Figure 3).
 220 If a given observation by NEON is reported as not passing a quality assurance check, we

221 applied a gap filling method to replace that measurement with its monthly mean at that same
222 depth (Section 4.2.1). Belowground measurements of soil water and soil temperature are then
223 interpolated to the same depth as soil CO₂ measurements. The diffusivity (Section 4.2.2) and
224 soil flux across different soil layers (Section 4.2.3) are then computed.

225 The third and final step is computing a surface soil flux through extrapolation to the surface
226 (purple parallelogram in Figure 2 and Panel c in Figure 3). Uncertainty on a soil flux
227 measurement is computed through quadrature. An aggregate quality assurance (QA) flag for
228 each environmental measurement is also reported, representing if any gap-filled measurements
229 were used in the computation of a soil flux. Within the soil flux-gradient method, several
230 different approaches can be used to derive a surface flux (Maier & Schack-Kirchner, 2014); the
231 `neonSoilFlux` package reports four different possible values for soil surface flux (Section 4.2.3)
232 for each of two different methods of diffusivity estimation, for a total of eight estimates of
233 flux.

234 4.2.1 Gap-filling routine

235 NEON reports QA flags as binary values for each measurement and half-hourly interval. For a
236 given half-hour, if any input variable (soil CO₂ concentration, soil temperature, or soil moisture)
237 at depth z is flagged, computation of F_S is not possible. To address this, flagged measurements
238 and their uncertainties were replaced with a bootstrapped monthly mean (\bar{m}) and monthly
239 standard deviation (\bar{s}) (Efron & Tibshirani, 1994).

240 For each month, depth z , and variable, we computed bootstrapped estimates of \bar{m} and \bar{s}
241 from the vectors of unflagged measurements (**m**), reported standard errors (σ), and the 95%
242 confidence interval (ϵ , or expanded uncertainty; Farrance & Frenkel (2012)). We also defined a

243 bias vector $\mathbf{b} = \sqrt{\epsilon^2 - \sigma^2}$, which quantifies the spread of uncertainty in a given period and is
244 incorporated into \bar{m} .

245 From these, 5000 bootstrap samples were generated for \mathbf{m} , σ , and \mathbf{b} . For each sample (m_k, b_k, σ_k) ,
246 we generated a vector \mathbf{n} (length $N = 5000$) by drawing from a normal distribution with mean
247 $m_k + b_k$ and standard deviation σ_k . The sample mean and standard deviation were then
248 computed from \mathbf{n} . The resulting distributions of sample means and sample standard deviations
249 provided the bootstrapped monthly mean (\bar{m}) and standard error (\bar{s}) respectively.

250 This gap-filling procedure provides a consistent treatment across all data streams. However,
251 alternative approaches may be better suited for longer gaps (e.g., correlations with other NEON
252 measurement levels or soil plots) or for variable-specific conditions. We discuss the effect of
253 gap-filling on our results in Section 6.1.

254 **4.2.2 Soil diffusivity**

255 Soil diffusivity D_a at a given measurement depth is the product of the diffusivity in free air
256 $D_{a,0}$ ($\text{m}^2 \text{ s}^{-1}$) and the tortuosity ξ (no units) (Millington & Shearer, 1971).

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

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

258 where T_i is soil temperature ($^\circ\text{C}$) at depth i (NEON, 2024d) and P surface barometric pressure
259 (kPa) (NEON, 2024a).

260 Previous studies by Sallam et al. (1984) and Tang et al. (2003) demonstrated the sensitivity
261 of modeled F_S depending on the tortuosity model (ξ) used to compute diffusivity. At low

262 soil water content, the choice of tortuosity model can lead to order-of-magnitude differences
263 in D_a , which in turn affect modeled F_S . The `neonSoilFlux` package currently includes two
264 approaches to calculate ξ , representing the range of tortuosity behavior reported in Sallam et
265 al. (1984).

266 The first approach is the Millington-Quirk model (Millington & Shearer, 1971), in which
267 tortuosity depends on both porosity and soil water content:

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

268 In Equation 2, SWC is the soil water content at depth i (NEON, 2024e) and ϕ is the porosity,
269 which in turn is a function of soil physical properties (NEON, 2024c):

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

270 In Equation 3, ρ_m is the particle density of mineral soil (2.65 g cm^{-3}), ρ_s the soil bulk density
271 (g cm^{-3}) excluding coarse fragments greater than 2 mm (NEON, 2024c), and f_V is a site-specific
272 value that accounts for the proportion of soil fragments between 2-20 mm. Soil fragments
273 greater than 20 mm were not estimated due to limitations in the amount of soil that can be
274 analyzed (NEON, 2024c). We assume that rock fragments contain no internal pores.

275 The Millington-Quirk model assumes ξ is modulated by the amount of fluid saturation in soil
276 pores (Millington & Shearer, 1971). In contrast, the Marshall model (Marshall, 1959) expresses
277 tortuosity as only a function of porosity ($\xi = \phi^{1.5}$), with ϕ defined from Equation 3. The
278 Marshall model is independent of soil water content and assumes tortuosity is only governed
279 by soil structure. The `neonSoilFlux` package allows users to choose the tortuosity model most
280 appropriate for site-specific conditions and research goals.

281 **4.2.3 Soil flux computation**

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

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

284 where D_a is the diffusivity ($\text{m}^2 \text{s}^{-1}$) and $\frac{dC}{dz}$ is the gradient of CO_2 molar concentration (μmol
285 m^{-3} , so the gradient has units of $\mu\text{mol m}^{-3} \text{m}^{-1}$). The soil surface flux is theoretically defined
286 by applying Equation 4 to measurements collected at the soil surface and directly below the
287 surface. Measurements of soil temperature, soil water content, and soil CO_2 molar concentration
288 across the soil profile allow for application of Equation 4 across different soil depths. Each
289 site had three measurement layers, so we denote the flux as a three-digit subscript F_{ijk} with
290 indicator variables i , j , and k indicate if a given layer was used (written in order of increasing
291 depth), according to the following:

- 292 • F_{000} is a surface flux estimate using the intercept of the linear regression of D_a with
293 depth and the slope from the linear regression of CO_2 with depth (which represents $\frac{dC}{dz}$
294 in Fick's Law). Tang et al. (2003) used this approach to compute fluxes in an oak-grass
295 savannah.
- 296 • F_{110} is a flux estimate across the two shallowest measurement layers.
- 297 • F_{011} is a flux estimate across the two deepest measurement layers.
- 298 • F_{101} is a flux estimate across the shallowest and deepest measurement layers.

299 For F_{110} , F_{011} , and F_{101} , the diffusivity used in Fick's Law is always at the deeper measurement
300 layer. When used as a surface flux estimate we assume CO_2 remains constant above this flux
301 depth. Uncertainty in all F_{ijk} values was quantified using quadrature (Taylor, 2022). These

302 computed fluxes could provide the basis for additional soil flux estimates. For example, Tang et
303 al. (2005) estimated surface flux by linearly extrapolating F_{110} and F_{011} to the soil surface.

304 **4.3 Post processing evaluation**

305 Following collection of field measurements and calculation of the soil fluxes from `neonSoilFlux`
306 package, we compared measured F_S based on closed-dynamic chamber measurements with the
307 LI-COR instruments to a given soil flux calculation from `neonSoilFlux` for each site and flux
308 computation method and quantified the relationship statistically (R^2). Finally, for a half-hourly
309 interval we also computed a *post hoc* diffusivity (D_a) using the LI-COR flux along with the
310 CO_2 surface gradient reported by NEON using the measurement levels closest to the surface.

311 **5 Results**

312 **5.1 Concordance between modelled and measured soil CO_2 flux**

313 The sites we visited ranged substantially in both their annual average temperature and
314 precipitation as well as their biome type (Table 2). These differences also influenced the wide
315 range of observed flux rates across sites.

316 The timeseries of the measured fluxes from the LI-COR 6800 and 870/8250 were compared
317 to modeled soil fluxes from the `neonSoilFlux` R package (Figure 4). We also assessed year-
318 long estimated flux time series and compared those to field measurements made at each site
319 (Figure 5). Results are reported in local time. Where applicable, sites are displayed from left
320 to right by increasing soil temperature (Table 1). Positive values of the flux indicate that there
321 is a flux moving towards the surface. Overall, with the exception of SRER (discussed later) the
322 computed fluxes determined using a variety of plausible methods spanned the field-measured

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

323 fluxes, but the specific flux-gradient method that best approximated field measurements varied
324 by site.

325 We calculated a statistical relationship between the various estimates of soil flux computed by
326 `neonSoilFlux` and the field-measured fluxes within daily interval periods. Statistics for these
327 comparisons are reported in Figure 6, which also shows how these fall relative to a 1:1 line.

328 5.2 Effects of method choice on diffusivity estimates

329 In four of six field sites, the *post hoc* D_a estimate fell roughly between the two diffusion
330 estimation methods; however this was less the case in the two driest sites, SJER and SRER
331 (Table 1), where the field estimate of diffusivity was either lower or higher than both of the
332 other methods (Figure 7).

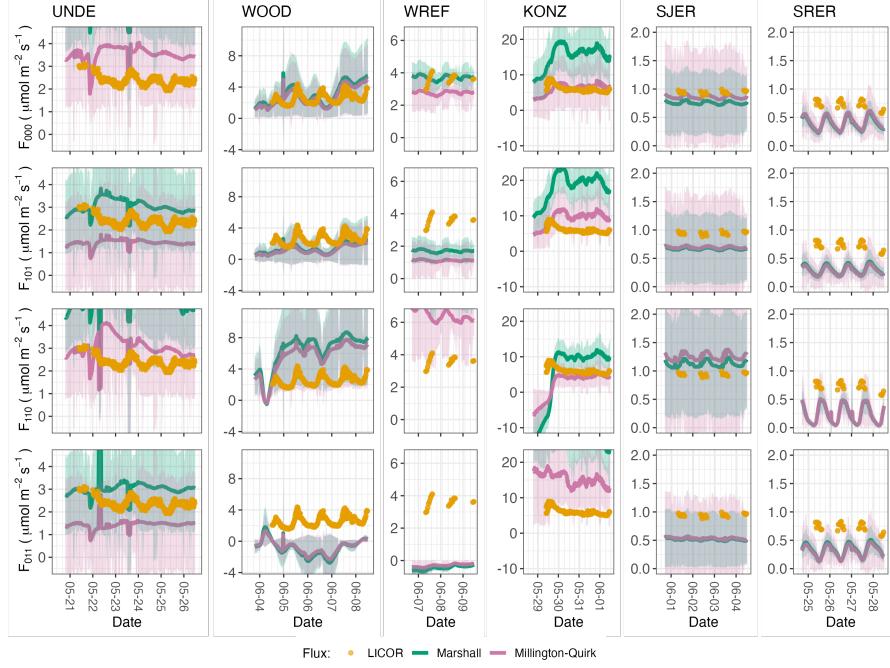


Figure 4: Timeseries of soil surface flux (F_S) from field-measured (yellow lines) and modeled soil fluxes (green or purple lines) by the `neonSoilFlux` R package. Fluxes from the `neonSoilFlux` R package are separated by the diffusivity model used (Millington-Quirk or Marshall, Section 4.2.2). Individual 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. WREF, SJER, and SRER were sampled in 2022, and UNDE, WOOD, and KONZ were sampled in 2024. Sites (columns) are arranged from left to right in terms of increasing mean annual temperature.

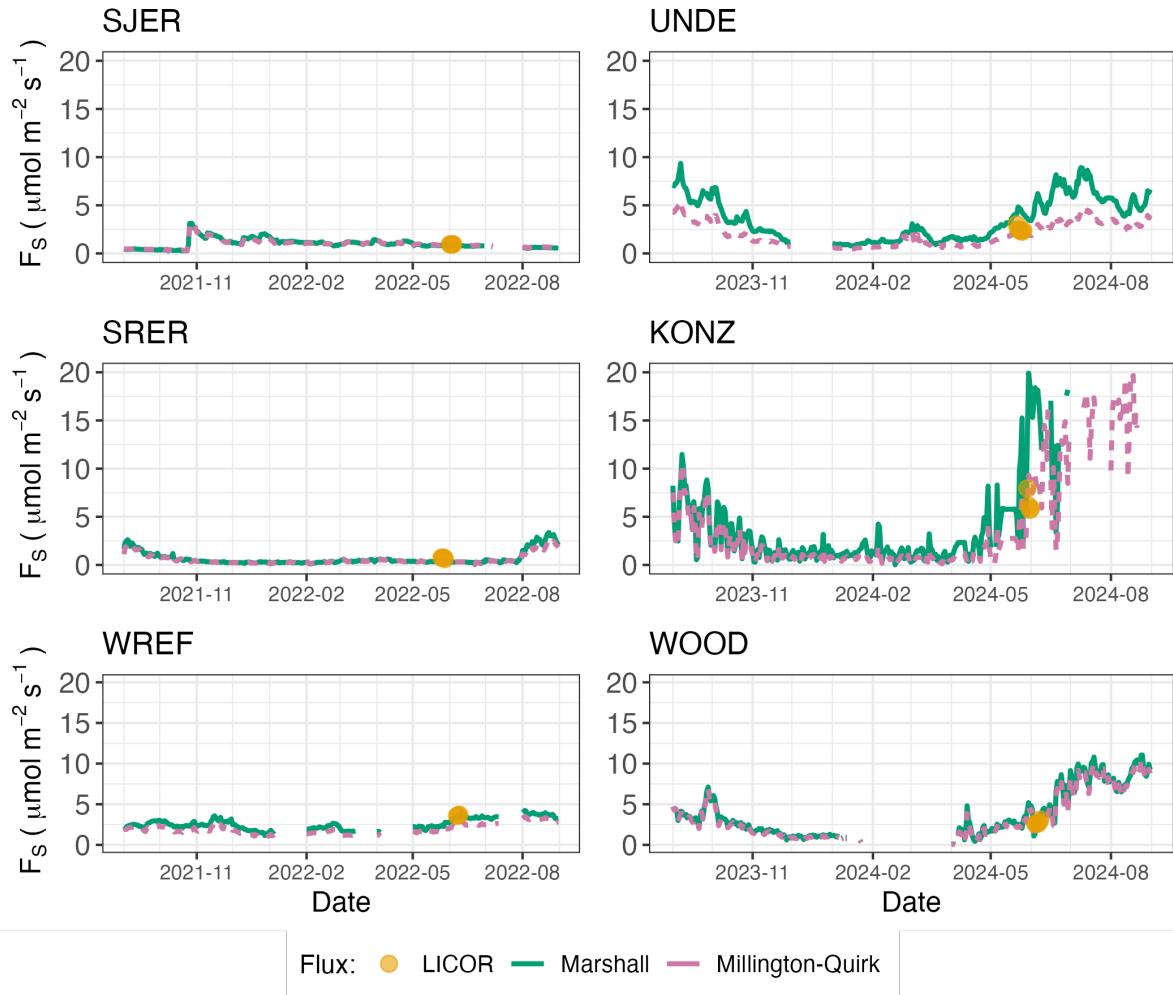


Figure 5: Timeseries of both daily-averaged field F_S (yellow circles) and daily ensemble averaged soil fluxes (average of F_{000} , F_{101} , F_{011} , F_{110} , Section 4.2.3) by the `neonSoilFlux` R package, separated by the diffusivity model used (green or purple lines, Millington-Quirk or Marshall,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

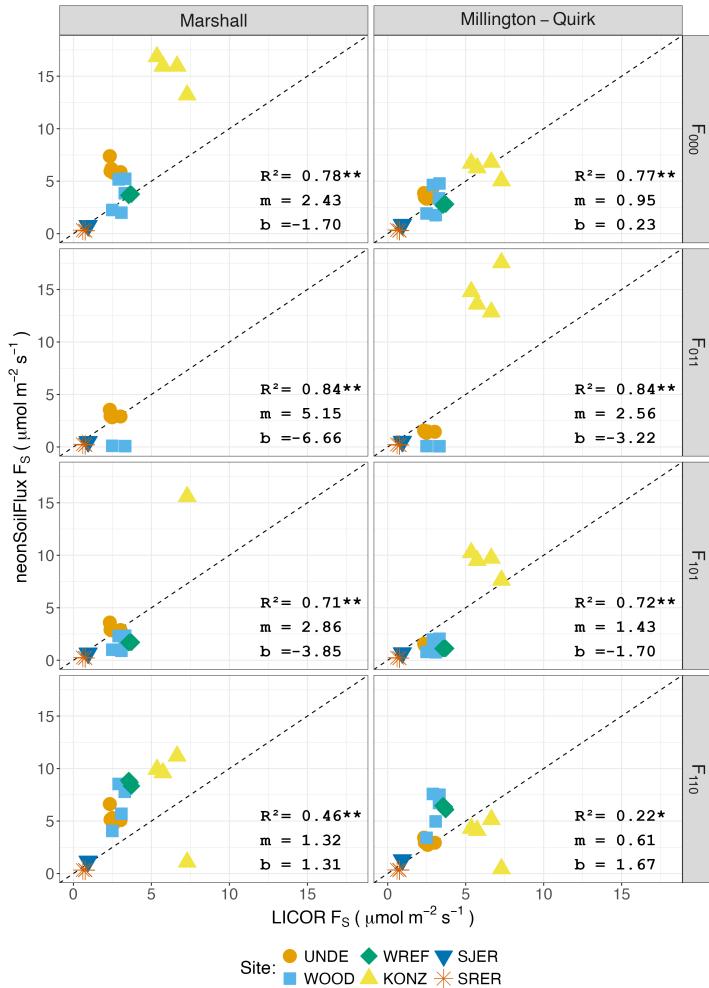


Figure 6: Statistical comparison between measured fluxes at each NEON site with fluxes reported by `neonSoilFlux` with the different flux calculation approaches and diffusivity calculations applied. Points are daily averages and LICOR F_S values are from the 6800 instrument only, for consistency. The dotted line represents a 1:1 relationship, and the reported R^2 quantifies the relationship between field-measured and `neonSoilFlux` estimated fluxes. * = significance at the 5% level, ** = significance at the 1% level. The slope (m) and intercept (b) of the linear regression between measured and modeled fluxes are also reported. The low-value outlier from KONZ in the F_{110} Marshall plot is an example of the effect of inverted CO_2 gradients causing an estimated flux to be negative, bringing down the daily mean, which later resolved as the soils dried back out. Intervals where calculated fluxes were < 0 ($n = 12$) were excluded from the plot; 3 each from WREF and WOOD when using (F_{011} approach).

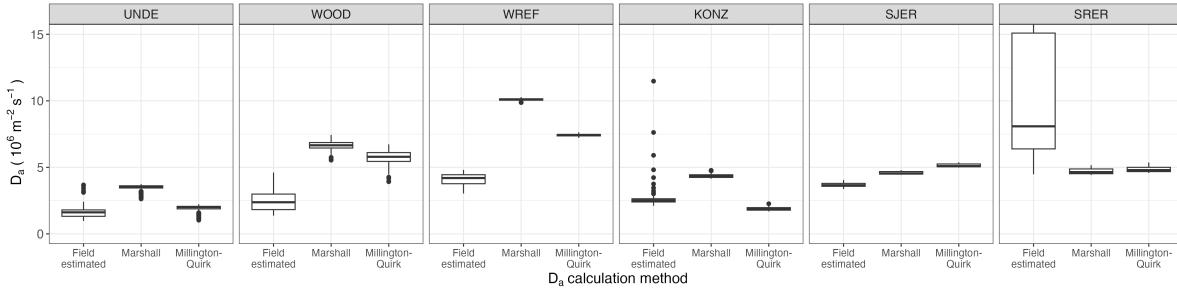


Figure 7: Distribution of diffusivity (D_a) at each study site. Values of D_a were provided by the `neonSoilFlux` package, computed from the Millington-Quirk or Marshall models (Section 4.2.2). A post-hoc estimate of diffusivity (labeled as “Field estimated”) was computed through the field measured flux (Figure 4), divided by the CO₂ 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. Some outliers (n = 2 from the field estimated values at KONZ and n = 9 from field estimated values at SRER) are excluded from the plot to allow better comparative visualization across sites.

333 6 Discussion

334 This study presents a unified data science workflow to efficiently process automated measure-
 335 ments of belowground soil CO₂ concentrations, soil water content, and soil temperature to
 336 infer estimates of soil surface CO₂ effluxes through application of Fick’s Law (Equation 4).
 337 Our core goals in this study were: (1) to generate estimates of soil flux from continuous soil
 338 sensor data at terrestrial NEON sites using the flux-gradient method and then (2) to compare
 339 those estimates to field-measured fluxes based on the closed chamber approach at six NEON
 340 focal sites. We discuss our progress toward these core goals through (1) an overall evaluation
 341 of the flux-gradient approach (and uncertainty calculation) and (2) site-specific evaluation of
 342 differences in estimated vs measured fluxes.

343 **6.1 General evaluation of flux-gradient approach**

344 Key assumptions of the flux-gradient approach are that CO₂ concentrations increase throughout
345 the soil profile such that the highest concentrations are observed in the deepest layers. Addition-
346 ally, field flux measurements should correlate with F_{000} because they represent surface fluxes.
347 Periods where this gradient condition are not met generally are connected to processes that occur
348 during soil wetting events, where more shallow soil layers produce higher concentrations of CO₂
349 due to microbial respiration pulses following rewetting. This effect is likely to be largest at sites
350 with rich organic soils (e.g. KONZ). Based on this reasoning, in these types of situations we would
351 *a priori* expect F_{011} (deepest layers) $\leq F_{101} \leq F_{110}$ (shallow layers) $\leq F_{000}$ (all layers) be-
352 cause the previous flux estimates rely primarily on CO₂ concentrations at deeper depths, and
353 could miss high concentrations of CO₂ produced in shallower layers.

354 When modeling soil respiration, typically a non-linear response function that also considers soil
355 type is used (Bouma & Bryla, 2000; Yan et al., 2016, 2018). For the `neonSoilFlux` package,
356 soil type is connected to the measurement of bulk density, which was characterized at each
357 NEON site. This bulk density estimate is based on replicate samples collected from the site
358 megapit at a subset of soil horizons, with an estimated uncertainty of $\pm 5\%$ (NEON, 2024c).
359 Coarse fragment estimates also have very large uncertainties, but because the volume fraction
360 tends to be low in surface soils it is unlikely to contribute much additional flux uncertainty.

361 Our results suggest that the most important way to improve reliability of the flux estimate is
362 to reduce the usage of gap-filled data. The current approach to gap filling in `neonSoilFlux`
363 uses monthly mean data to gap fill—this approach decreases the ability of the estimate to be
364 responsive to short-term pulses that occur with rapid weather shifts. Four sites (KONZ, SRER,
365 WREF, and UNDE) had more than 75% of half-hourly periods with no-gap filled measurements
366 (Figure S1, Supplementary Information). Two sites (SJER and WOOD) had more than 75% of
367 half-hourly intervals with just one gap-filled measurement. The large uncertainty evident in

368 Figure 4 for estimates from WOOD and SJER are thus due in part to the gap-filling used in
369 these sites (Figure S1). While we did not need to use gap-filled measurements to compute the
370 flux at WREF, field data collection occurred following a severe rainstorm, with soils at the
371 beginning of the sampling week near their water holding capacity. In general, we recommend
372 that whenever possible, knowledge of local field conditions should influence analysis decisions
373 in addition to any QA filtering protocols in the `neonSoilFlux` package.

374 We recognize that this gap-filling approach may lead to gap-filled values that are quite different
375 from the actual values, such as an underestimate of soil moisture following rain events. Further
376 extensions of the gap filling method could use more sophisticated gap-filling routines, similar to
377 what is used for net ecosystem carbon exchange (Falge et al., 2001; Liu et al., 2023; Mariethoz
378 et al., 2015; Moffat et al., 2007; Zhang et al., 2023). Additionally, since the deepest temperature
379 and soil moisture sensors are located below the deepest CO₂ sensors at NEON sites, it is
380 possible that excluding these deeper layers from consideration prior to analysis would lead to a
381 reduced need for gap filling. Future iterations of the `neonSoilFlux` package may incorporate
382 this as an option. The current gap-filling routine provides a consistent approach that can be
383 applied to each data stream, but further work may explore alternative gap-filling approaches.

384 **6.2 Evaluation of flux-gradient approach at each site**

385 Derived results from the `neonSoilFlux` package have patterns that are broadly consistent with
386 those directly measured in the field (Figure 4 and Figure 5), even though statistical comparisons
387 between the field-measured and `neonSoilFlux` values were quite variable (e.g. R^2 ranging
388 from 0.04 to 0.81; Figure 6). One advantage of the `neonSoilFlux` package is its ability to
389 calculate fluxes across different soil depths (Figure 3), which allows for additional site-specific
390 customization. We believe the package can provide a useful baseline estimate of soil fluxes that
391 can always be complemented through additional field measurements.

392 The six locations studied provide a range of case studies that suggest different considerations
393 may apply to different sites when applying the flux-gradient method. For example, the Santa
394 Rita Experimental Range (SRER) is a desert site characterized by sandy soil, which also was
395 the location of the highest field soil temperatures that we observed (Table 2). At SRER the
396 flux across the top two layers (F_{110}) produced a pattern of soil flux most consistent with the
397 observed field data. The remaining methods F_{101} , F_{011} , or F_{000} are derived from information
398 taken from the deepest layer, which seems to have been decoupled from the surface layers both
399 in terms of temperature and CO₂ concentration. This may be a general circumstance where
400 there are large diurnal temperature extremes that rapidly change during the course of a day
401 and overnight, leading to lags in the timing of when temperature increases propagate down to
402 deeper soil layers.

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

409 Both of the previous cases also provide context for the variable statistical comparisons between
410 field-measured soil fluxes and `neonSoilFlux` outputs (Figure 6). When considering systematic
411 deployment of this method across a measurement network, there are a number of independent
412 challenges that require careful consideration. There are clear tradeoffs between (1) accuracy of
413 modeled fluxes (defined here as closeness to field-measured F_S and the uncertainty reduction
414 factor ϵ), (2) precision (which could be defined by the signal to noise ratio), and (3) the
415 choice of the diffusivity model (Section 4.2.2) or flux computation method (Section 4.2.3). A
416 sensitivity analysis (Figure S2, Supplemental Information) found that flux output uncertainty

417 was dominated by measurement uncertainty (T_S , P , SWC , or CO_2) rather than by the diffusivity
418 method used to compute soil flux. Notably, the F_{110} method was least sensitive to measurement
419 uncertainty likely because it best aligns with the surface chamber measurement assumptions.

420 Finally, comparing the effects of different diffusivity estimation methods on the match between
421 modeled and measured fluxes (Figure 5) highlights the sensitivity of F_{ijk} to diffusivity. The
422 comparison between diffusivity estimates compared to field estimated diffusivity (Figure 7)
423 demonstrates that site parameters can dictate which measure of diffusivity is most likely to be
424 accurate in a given environmental context. Site-specific differences are largely a reflection of
425 differences in soil moisture across the sites (Table 1), as not all diffusivity estimation methods
426 incorporate soil moisture equivalently. While we here have compares two approaches to calculate
427 diffusivity (the Millington-Quirk and Marshall models), it may be valuable to evaluate other
428 diffusivity models (e.g. the Moldrup model; Moldrup et al. (1999)) as well. Ultimately the
429 choice of a particular diffusivity model could be determined based on knowledge of site-specific
430 evaluations or a set of these models could be used to generate a model ensemble average as a
431 means to trade precision for a more general approach.

432 **6.3 Recommendations for future method development**

433 The `neonSoilFlux` package provides several approaches to estimate soil flux using the gradient
434 method. We believe these approaches enable the software to be used across a range of site-
435 specific assumptions (Maier & Schack-Kirchner, 2014). We note, however, that this choice
436 can have a determinative approach on the calculated values. Ensemble averaging approaches
437 (Elshall et al., 2018; Raftery et al., 2005) may be one way to address this problem if the goal is
438 to calculate fluxes using the same method at a diverse range of different sites. Two other ideas
439 would be to apply machine learning algorithms (e.g. random forest) to generate a single flux
440 estimate across diverse sites, or using co-located estimates of net ecosystem carbon exchange

⁴⁴¹ from eddy-flux towers to further constrain results or to assess soil flux results for plausibility
⁴⁴² (Phillips et al., 2017).

⁴⁴³ These challenges notwithstanding, the method used here and made available in the
⁴⁴⁴ `neonSoilFlux` R package has the potential to produce nearly continuous estimates of flux
⁴⁴⁵ across all terrestrial NEON sites. These estimates are a significant improvement on available
⁴⁴⁶ approaches to constrain the portion of ecosystem respiration attributable to the soil. This, in
⁴⁴⁷ turn, also aids in our ability to understand the soil contribution to the net ecosystem flux
⁴⁴⁸ measured at these sites using the co-located eddy flux towers.

⁴⁴⁹ 7 Conclusions

⁴⁵⁰ We used the R package `neonSoilFlux` to estimate soil CO₂ fluxes with the flux-gradient method
⁴⁵¹ using data from buried soil sensors at NEON terrestrial sites. We compared the predicted
⁴⁵² fluxes to those measured directly using a field-based closed chamber approach. Soil fluxes
⁴⁵³ from `neonSoilFlux` were broadly effective at producing estimates of flux comparable to those
⁴⁵⁴ measured in the field using a chamber-based technique. However `neonSoilFlux` outputs are
⁴⁵⁵ quite sensitive to a number of issues, including: missing data (and thus gap-filling of input
⁴⁵⁶ measurement datasets), the selection of soil depths used to best calculate the gradient (which
⁴⁵⁷ may vary between sites), and finally the choice of method used for estimating soil diffusivity.
⁴⁵⁸ The flexibility of the `neonSoilFlux` package allows the user to evaluate each of these issues
⁴⁵⁹ with site-specific knowledge and contexts. Future refinements and subsequent validation of
⁴⁶⁰ `neonSoilFlux` outputs will feed forward into evaluating soil carbon fluxes broader spatial scales
⁴⁶¹ to enhance understanding of the ways in which soils across diverse ecosystems are responding
⁴⁶² to a changing climate.

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