

**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**

**6      John Zobitz<sup>1</sup>      Ed Ayres<sup>2</sup>      Zoey Werbin<sup>3</sup>      Ridwan Abdi<sup>1</sup>**

**7      Natalie Ashburner-Wright<sup>4</sup>      Lillian Brown<sup>4</sup>**

**8      Ryan Frink-Sobierajski<sup>4</sup>      Lajntxiag Lee<sup>1</sup>      Dijonë Mehmeti<sup>1</sup>**

**9      Christina Tran<sup>4</sup>      Ly Xiong<sup>1</sup>      Naupaka Zimmerman<sup>4</sup>**

**10     <sup>1</sup> Augsburg University, 2211 Riverside Avenue, Minneapolis, MN 55454**

**11     <sup>2</sup> National Ecological Observatory Network, 1685 38th Street, Suite 100, Boulder, CO 80301**

**12     <sup>3</sup> Boston University, 5 Cummington Street, Boston, MA 02215**

**13     <sup>4</sup> University of San Francisco, 2130 Fulton Street, San Francisco, CA 94117**

<sup>14</sup> **Acknowledgments**

<sup>15</sup> JZ acknowledges Kathleen O'Rourke for code development. NZ thanks technical staff at  
<sup>16</sup> USF for support with field gear assembly and shipping. We thank the NEON field staff  
<sup>17</sup> and assignable assets teams for facilitating each of the six NEON site visits. We are grateful  
<sup>18</sup> to LI-COR technical staff for helpful discussions about optimal sampling methods. This work  
<sup>19</sup> was supported by NSF DEB grant #2017829 awarded to JZ, and NSF DEB grant #2017860  
<sup>20</sup> awarded to NZ.

<sup>21</sup> **Conflict of Interest Statements**

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

<sup>24</sup> **Author Contributions**

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

<sup>31</sup> **Data Availability**

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

<sup>34</sup> **1 Abstract**

<sup>35</sup> A key component of constraining the uncertainty of the terrestrial carbon sink is quantification  
<sup>36</sup> of terrestrial soil carbon fluxes, which vary across time and ecosystem type. One method for  
<sup>37</sup> the estimation of these fluxes and their associated uncertainties is the flux gradient method,  
<sup>38</sup> which can be calculated via a variety of existing approaches. Robust estimation of soil carbon  
<sup>39</sup> fluxes on a sub-daily level requires measurements of soil CO<sub>2</sub> concentration, water content,  
<sup>40</sup> temperature, and other environmental measurements and soil properties. These data are  
<sup>41</sup> publicly available from the National Ecological Observatory Network at sites spanning a range  
<sup>42</sup> of 20 different ecoclimatic domains across the continental United States, Puerto Rico, Alaska,  
<sup>43</sup> and Hawai'i. We present an R software package (`neonSoilFlux`) that acquires NEON soil  
<sup>44</sup> environmental data and computes soil carbon flux at a half-hourly time step at a user-specified  
<sup>45</sup> NEON site and month in a tidy data format. To validate the computed fluxes, we visited six  
<sup>46</sup> focal NEON sites and measured soil carbon fluxes using a closed-dynamic chamber approach.  
<sup>47</sup> The validation confirmed that a primary challenge in reducing soil carbon flux uncertainty is  
<sup>48</sup> correctly characterizing diffusivity and soil water content across the soil profile. Outputs from  
<sup>49</sup> the `neonSoilFlux` package contribute to existing databases of soil carbon flux measurements,  
<sup>50</sup> providing near real-time estimates of a critical component of the terrestrial carbon cycle.

<sup>51</sup> **1.1 Keywords**

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

<sup>54</sup> **2 Data for peer review**

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

<sup>56</sup> **3 Introduction**

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

<sup>68</sup> Ecological observation networks such as the United States' National Ecological Observatory  
<sup>69</sup> Network (NEON) and others (e.g. FLUXNET or the Integrated Carbon Observation System)  
<sup>70</sup> present a significant advancement in the nearly continuous observation of biogeochemical pro-  
<sup>71</sup> cesses at the continental scale. Notably, at 47 terrestrial sites across the continental United  
<sup>72</sup> States, NEON provides half-hourly measurements of soil CO<sub>2</sub> concentration, temperature,  
<sup>73</sup> and moisture at different vertical depths. Each of these NEON sites also encompasses mea-  
<sup>74</sup> surements of the cumulative sum of all ecosystem carbon fluxes in an airshed using the eddy  
<sup>75</sup> 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  $\text{CO}_2$  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  $\text{CO}_2$  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 CO<sub>2</sub> 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.

<sub>121</sub> **4 Materials and Methods**

<sub>122</sub> **4.1 Field methods**

<sub>123</sub> **4.1.1 Focal NEON Sites**

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

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

<sub>132</sub> **4.1.2 Soil collar placement**

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

<sup>139</sup> **4.1.3 Infrared gas analyzer measurements of soil CO<sub>2</sub> flux**

<sup>140</sup> In 2022, we then made measurements of flux on an hourly interval for 8 hours each day.  
<sup>141</sup> Measurements were taken from roughly 8 am to 4 pm, with the time interval selected to  
<sup>142</sup> capture the majority of the diurnal gradient of soil temperature each day. These measurements  
<sup>143</sup> were made using a LI-6800 infrared gas analyzer instrument (LI-COR Environmental, Lincoln,  
<sup>144</sup> NE) fitted with a soil chamber attachment (attachment 6800-09). In 2024, we again used  
<sup>145</sup> the same LI-6800 instrument, but made half-hourly measurements over an approximately 8  
<sup>146</sup> hour period. In addition, we also installed a second collar and used a second instrument, an  
<sup>147</sup> LI-870 CO<sub>2</sub> IRGA, connected to an automated robotic chamber (LI-COR chamber 8200-104)  
<sup>148</sup> controlled by an LI-8250 multiplexer, to make automated measurements. The multiplexer was  
<sup>149</sup> configured to take half-hourly measurements 24 hours a day for the duration of our sampling  
<sup>150</sup> bout at each site. Each instrument was paired with a soil temperature and moisture probe  
<sup>151</sup> (Stevens HydraProbe, Stevens Water, Portland, OR) that was used to make soil temperature  
<sup>152</sup> and moisture measurements concurrent with the CO<sub>2</sub> flux measurements. Chamber volumes  
<sup>153</sup> were set by measuring collar offsets at each site. System checks were conducted daily for the  
<sup>154</sup> LI-6800 and weekly for the LI-8250. Instruments were factory calibrated before each field  
<sup>155</sup> season.

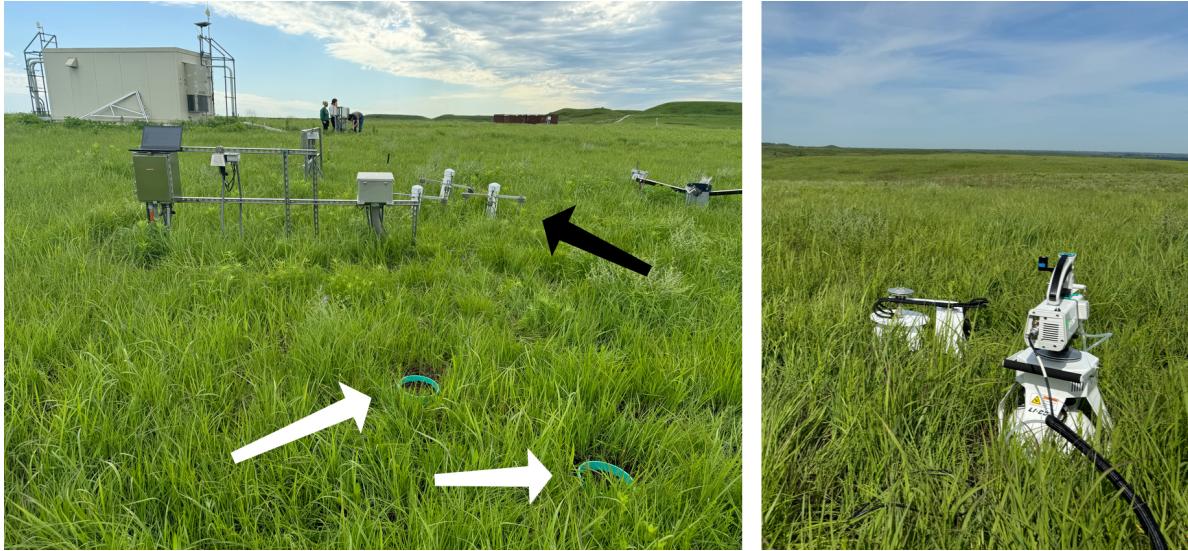


Figure 1: Spatial layout of field sampling using a closed-dynamic chamber setup at a representative NEON site (KONZ). Left image shows collars (white arrows) and permanent soil sensor installation (black arrow) and right image shows the LI-6800 (foreground) and LI-8200-104 (background) instruments placed 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 Environmental Research Center (UNDE)	46.23391, - 89.537254	Deciduous forest	4.3°	13.0°	802 mm	13.0%	22 May 2024 - 25 May 2024	004

#### 156 4.1.4 Post-collection processing of data

157 We used LI-COR SoilFluxPro software (v 5.3.1) to assess the appropriateness of dead band  
 158 and measurement duration using built-in evaluation tools. The deadband was set for 30-40  
 159 seconds, depending on the site, and the measurement duration was 180 seconds with a 30  
 160 second pre-purge and a 30 second post-purge.

#### 161 4.2 neonSoilFlux R package

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

166 (<https://CRAN.R-project.org/package=neonUtilities>). Figure 2 outlines the basic workflow  
167 of the package.

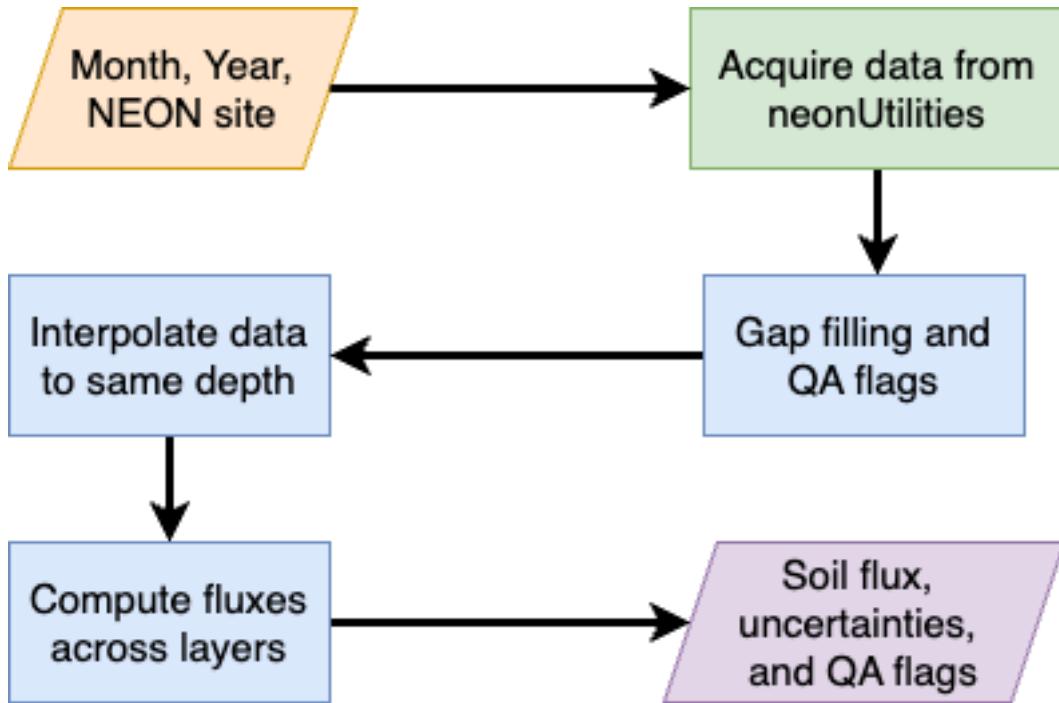


Figure 2: Diagram of `neonSoilFlux` R package. For a given month, year and NEON site (orange parallelogram), the package acquires all relevant data to compute  $F_S$  using the `neonUtilities` R package (green rectangle). Data are gap-filled according to reported QA flags and interpolated to the same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

168 At a given NEON observation there are five replicate soil plots, each with measurements of  
169 soil  $\text{CO}_2$  concentration, soil temperature, and soil moisture at different depths (Figure 3). The  
170 `neonSoilFlux` package acquires measured soil water content (National Ecological Observatory  
171 Network (NEON), 2024e), soil  $\text{CO}_2$  concentration (National Ecological Observatory Network  
172 (NEON), 2024b), barometric pressure from the nearby tower (National Ecological Observa-  
173 tory Network (NEON), 2024a), soil temperature (National Ecological Observatory Network  
174 (NEON), 2024d), and soil properties (e.g. bulk density) (National Ecological Observatory Net-

175 work (NEON), 2024c). The static soil properties were collected from a nearby soil pit during  
 176 site characterization and are assumed to be constant at each site.

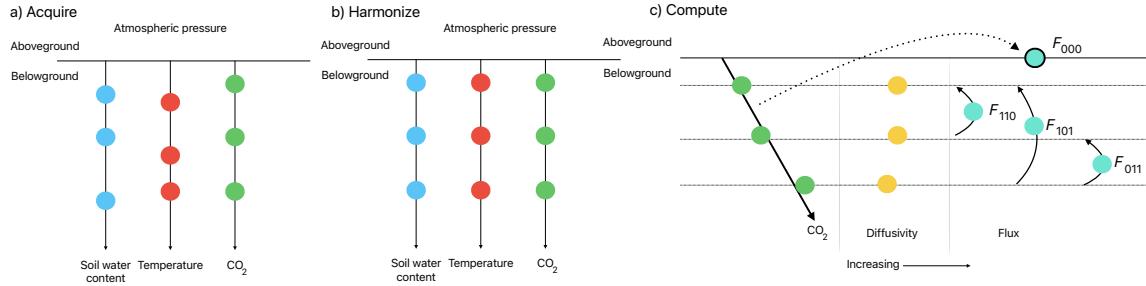


Figure 3: Model diagram for data workflow for the `neonSoilFlux` R package. a) Acquire: Data are obtained from given NEON location and horizontal sensor location, which includes soil water content, soil temperature, CO<sub>2</sub> concentration, and atmospheric pressure. All data are screened for quality assurance, with gap-filling of missing data reported. b) Any belowground data are then harmonized to the same depth as CO<sub>2</sub> concentrations using linear regression. c) The flux across a given depth is computed via Fick's law, denoted with  $F_{ijk}$ , where  $i$ ,  $j$ , or  $k$  are either 0 or 1 denoting the layers the flux is computed across ( $i$  = closest to surface,  $k$  = deepest).  $F_{000}$  represents a flux estimate where the gradient  $dC/dz$  is the slope of a linear regression of CO<sub>2</sub> with depth.

177 The workflow to computing a value of  $F_S$  with the `neonSoilFlux` consists of three primary  
 178 steps, illustrate in Figure 3. First, NEON data are acquired for a given site and month via the  
 179 `neonUtilities` R package (yellow parallelogram and green rectangle in Figure 2 and Panel a  
 180 in Figure 3). Acquired environmental data can be exported to a comma separated value file  
 181 for additional analysis. Quality assurance (QA) flags with an observation are reported as an  
 182 indicator variable.

183 The next step is harmonizing the data to compute soil fluxes across soil layers. This step  
 184 consists of three different actions (blue rectangles in Figure 2 and Panel b in Figure 3). If a  
 185 given observation by NEON is reported as not passing a quality assurance check, we applied  
 186 a gap filling method to replace that measurement with its monthly mean at that same depth  
 187 (Section 4.2.1). Belowground measurements of soil water and soil temperature are then inter-

188 polated to the same depth as soil CO<sub>2</sub> measurements. The diffusivity (Section 4.2.2) and soil  
189 flux across different soil layers (Section 4.2.3) are then computed.

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

#### 197 4.2.1 Gap-filling routine

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

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

- 206 1. Randomly sample from the uncertainty and bias independently:  $\sigma_j$  and the bias  $\mathbf{b}_k$  (not  
207 necessarily the same sample).
- 208 2. Generate a vector  $\mathbf{n}$  of length  $N$ , where  $\mathbf{n}_i$  is a random sample from a normal distribution  
209 with mean  $m_i$  and standard deviation  $\sigma_j$ . Since  $M < N$ , values from  $\mathbf{m}$  will be reused.

210 3. With these  $N$  random samples,  $\bar{y}_i = \bar{x} + \vec{b}_k$  and  $s_i$  is the sample standard deviation of  $\bar{x}$ .

211 We expect that  $s_i \approx \vec{\sigma}_j$ .

212 4. The reported monthly mean and standard deviation are then computed  $\bar{\bar{y}}$  and  $\bar{s}$ . Mea-

213 surements and uncertainties that did not pass the QA check are then substituted with

214  $\bar{\bar{y}}$  and  $\bar{s}$ .

215 This gap-filling method described here provides a consistent approach for each data stream,

216 however we recognize that other gap-filling alternatives may be warranted for longer-term gaps

217 (e.g. such as correlations with other NEON measurement levels and soil plots), or measure-

218 ment specific gap-filling routines. We discuss the effect of gap-filling on our measurements in

219 Section 6.

220 **4.2.2 Soil diffusivity**

221 Soil diffusivity  $D_a$  at a given measurement depth is the product of the diffusivity in free air

222  $D_{a,0}$  ( $\text{m}^2 \text{ s}^{-1}$ ) and the tortuosity  $\xi$  (no units) (Millington & Shearer, 1971).

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

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

224 where  $T_i$  is soil temperature ( $^\circ\text{C}$ ) at depth  $i$  (National Ecological Observatory Network

225 (NEON), 2024d) and  $P$  surface barometric pressure (kPa) (National Ecological Observatory

226 Network (NEON), 2024a).

227 Previous studies by Sallam et al. (1984) and Tang et al. (2003) demonstrated the sensitivity

228 of modeled  $F_S$  depending on the tortuosity model used to compute diffusivity. At low soil

229 water content, the choice of tortusosity model may lead to order of magnitude differences in  
 230  $D_a$ , which in turn affect modeled  $F_S$ . The `neonSoilFlux` package uses two different models  
 231 for  $\xi$ , representing the extremes reported in Sallam et al. (1984). The first approach uses the  
 232 Millington-Quirk model for diffusivity, Equation 2 (Millington & Shearer, 1971):

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

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

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

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

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

244 **4.2.3 Soil flux computation**

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

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

247 where  $D_a$  is the diffusivity ( $\text{m}^2 \text{s}^{-1}$ ) and  $\frac{dC}{dz}$  is the gradient of  $\text{CO}_2$  molar concentration  
248 ( $\mu\text{mol m}^{-3}$ , so the gradient has units of  $\mu\text{mol m}^{-3} \text{m}^{-1}$ ). The soil surface flux is theoretically  
249 defined by applying Equation 4 to measurements collected at the soil surface and directly  
250 below the surface. Measurements of soil temperature, soil water content, and soil  $\text{CO}_2$  molar  
251 concentration across the soil profile allow for application of Equation 4 across different soil  
252 depths. Each site had three measurement layers, so we denote the flux between which two  
253 layers as a three-digit subscript  $F_{ijk}$  with indicator variables  $i$ ,  $j$ , and  $k$  indicate if a given  
254 layer was used (written in order of increasing depth), according to the following:

- 255 •  $F_{000}$  is a surface flux estimate using the intercept of the linear regression of  $D_a$  with  
256 depth and the slope from the linear regression of  $\text{CO}_2$  with depth (which represents  $\frac{dC}{dz}$   
257 in Fick's Law). Tang et al. (2003) used this approach to compute fluxes in an oak-grass  
258 savannah.
- 259 •  $F_{110}$ ,  $F_{011}$  are fluxes across the two most shallow layers and two deepest layers respectively.  
260 The diffusivity used in Fick's Law is always at the deeper measurement layer.  
261 When used as a surface flux estimate we assume  $\text{CO}_2$  remains constant above this flux  
262 depth.
- 263 •  $F_{101}$  is a surface flux estimate using linear extrapolation using concentration measure-  
264 ments between the shallowest and deepest measurement layer. Hirano et al. (2003) and

265 Tang et al. (2005) used an approach similar to  $F_{101}$  in a temperate deciduous broadleaf  
266 forest and ponderosa pine forest respectively.

267 Uncertainty in all  $F_{ijk}$  is computed through quadrature (Taylor, 2022).

### 268 4.3 Post processing evaluation

269 Following collection of field measurements from the LICOR and calculation of the soil fluxes  
270 from `neonSoilFlux` package, we compared measured  $F_S$  (from the LICOR instruments) to a  
271 given soil flux calculation `neonSoilFlux` for each site and flux computation method. Statistics  
272 included the associated  $R^2$  value, root mean squared error (RMSE), and signal to noise ratio  
273 (SNR), defined as the ratio of a modeled soil flux ( $F_{ijk}$ ) from `neonSoilFlux` to its quadrature  
274 uncertainty ( $\sigma_{ijk}$ ).

275 We observed that the range of values (e.g.  $F_{ijk} \pm \sigma_{ijk}$ ) was much larger than the measured  
276 field flux. We evaluated  $|F_S - F_{ijk}| < (1 - \epsilon)\sigma_{ijk}$ , where  $F_S$  is a measured field soil flux  
277 from the LICOR 6800 (the LICOR 8250 was used at only three sites). The parameter  $\epsilon$  was  
278 an uncertainty reduction factor to evaluate how much the quadrature uncertainty could be  
279 reduced while maintaining precision between modeled  $F_{ijk}$  and measured  $F_S$ .

280 Finally, for a half-hourly interval we also computed a *post hoc*  $D_a$  using the LICOR flux along  
281 with the CO<sub>2</sub> surface gradient reported by NEON using the measurement levels closest to the  
282 surface.

283 **5 Results**

284 Figure 4 reports the timeseries of out the measured fluxes from the LICOR 6800 and 8250 com-  
 285 pared to modeled soil fluxes from the `neonSoilFlux` R package. Figure 5 and and computed  
 286 fluxes and uncertainty at each measurement site. Results are reported in local time. Positive  
 287 values of the flux indicate that there is a flux moving towards the surface. For ease of clarity  
 288 the fluxes at  $F_{111}$  and  $F_{000}$  are only shown in the top row (surface), followed by the fluxes at  
 289 individual separate layer ( $F_{100}$ ,  $F_{010}$ ,  $F_{001}$ ). Overall, with the exception of WREF and SRER  
 290 (discussed later) the computed fluxes were on the same order of magnitude and timing as the  
 291 measured field fluxes.

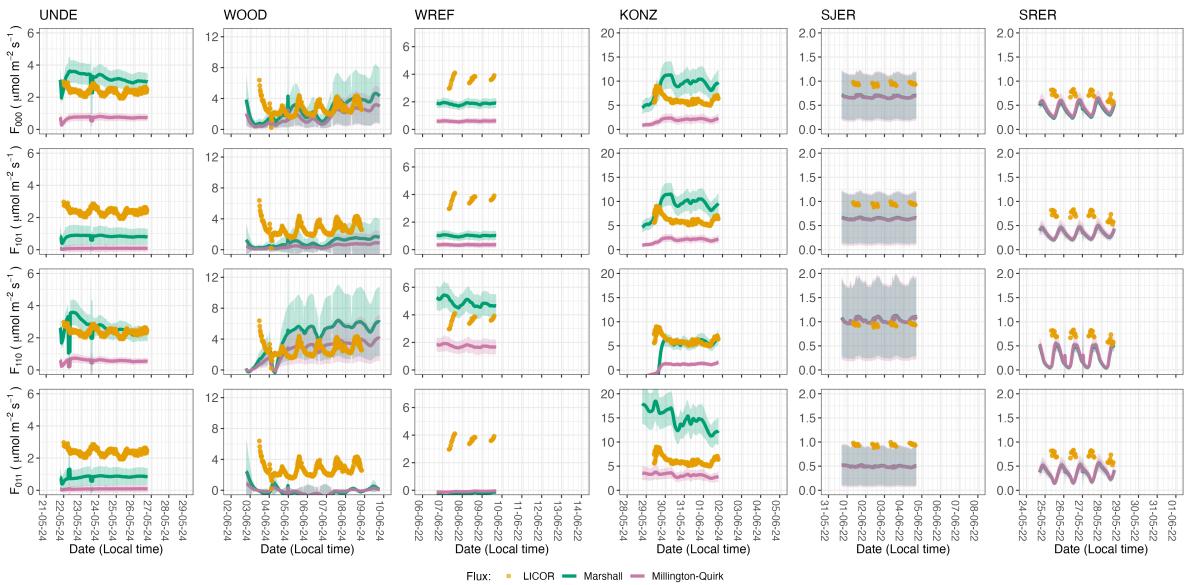


Figure 4: Timeseries of both measured  $F_S$  (yellow circles) and modeled soil fluxes (green or purple lines) by the `neonSoilFlux` R package. Fluxes from the `neonSoilFlux` R package are separated by the diffusivity model used (Millington-Quirk or Marshall, Section 4.2.2). Vertical axis labels in the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

292 For a given half-hourly time period, the `neonSoilFlux` packages assigns a QA flag for a mea-

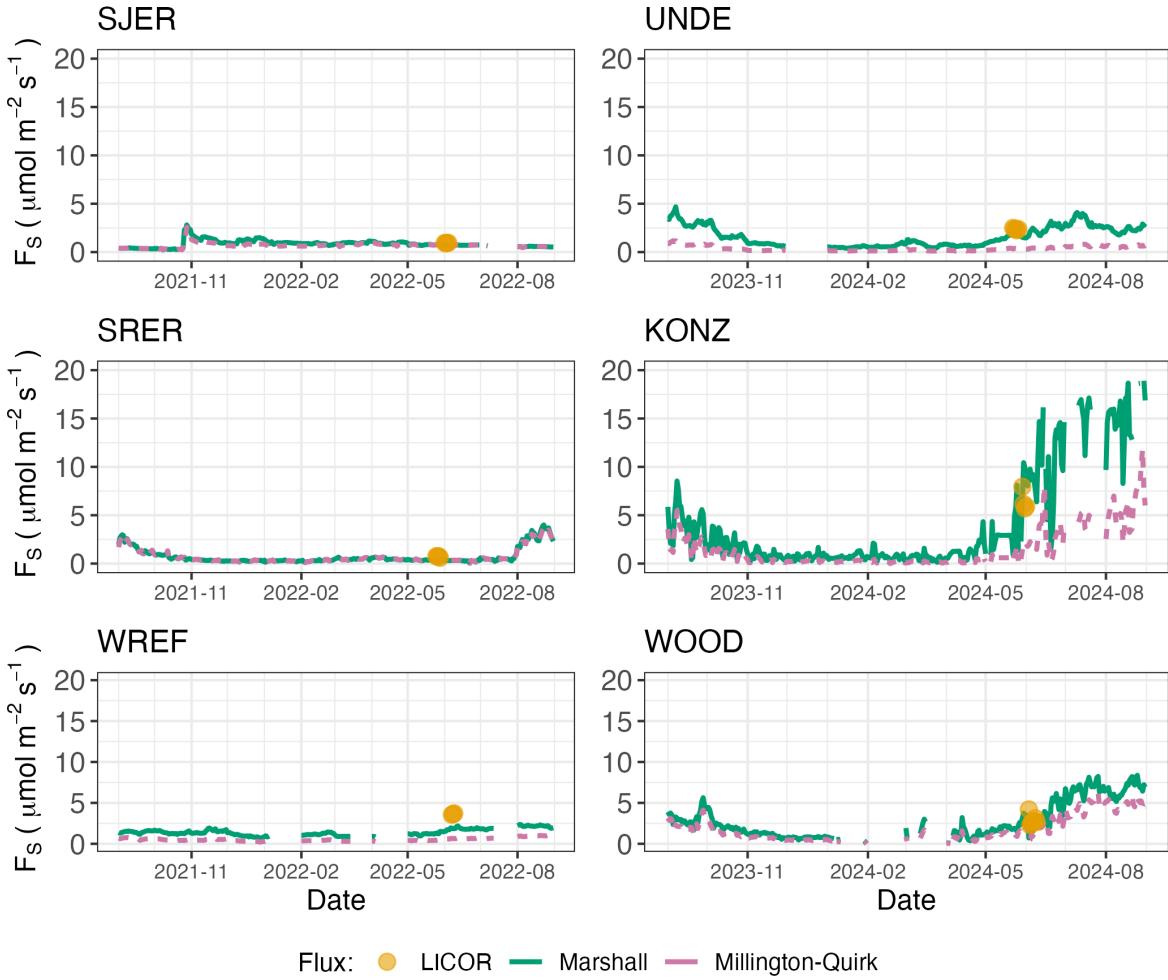


Figure 5: Timeseries of both daily-averaged field  $F_S$  (yellow circles) and daily ensemble averaged soil fluxes (green or purple lines) by the `neonSoilFlux` R package, separated by the diffusivity model used (Millington-Quirk or Marshall, Section 4.2.2). The time-series of modeled fluxes are a daily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

	Millington-Quirk		Marshall	
	NRMSE	R2	NRMSE	R2
<b>KONZ</b>				
$F_{110}$	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
<b>SJER</b>				
$F_{110}$	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
<b>SRER</b>				
$F_{110}$	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
<b>UNDE</b>				
$F_{110}$	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
<b>WOOD</b>				
$F_{110}$	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
<b>WREF</b>				
$F_{110}$	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

Figure 6

293 surement if more one values across all measurement depths uses gap-filled data (Section 4.2.1).  
 294 Panel a of Figure 7 reports the distribution for all input environmental measurements at each  
 295 site when field measurements were made. Soil fluxes are computed from 4 different types of  
 296 input measurements ( $T_S$ ,  $SWC$ ,  $P$ , and  $CO_2$ ), any of which could have a QA flag in a half-  
 297 hourly interval. Panel b of Figure 7 displays at each site the distribution of the number of  
 298 different gap-filled measurements used to compute a half-hourly flux. The largest contribution  
 299 to gap-filled measurements was soil water. SJER and WOOD utilized the largest number of  
 300 gap-filled measurements, which were primarily  $SWC$  and  $T_S$ .

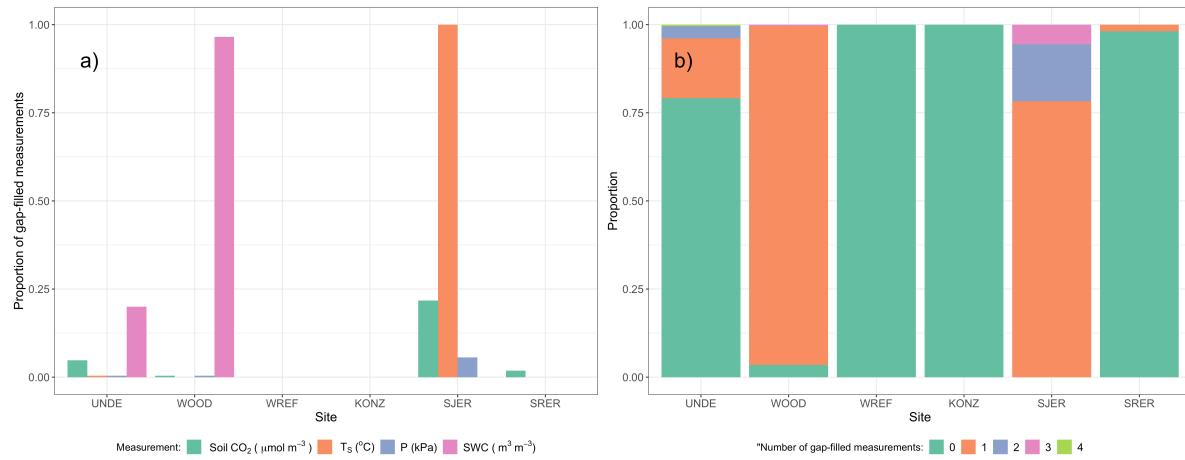


Figure 7: Panel a) Proportion of input gap-filled environmental measurements used to generate  $F_S$  from the `neonSoilFlux` package, by study site. Panel b) distribution of the usage of gap-filled measurements at each site.

301 Figure 8 reports both the computed SNR and the proportion of measured field fluxes within the  
 302 modeled uncertainty for a given flux computation method  $F_{ijk}$  (Section 4.3). Here, values of  
 303 SNR greater than unity indicates a reported uncertainty is smaller, propogated by quadrature  
 304 from a relatively higher precision from measured input variables ( $CO_2$ ,  $T_S$ ,  $SWC$ , or  $P$ ). The  
 305 sensitivity to the uncertainty reduction factor ( $\epsilon$ , bottom panels in Figure 8) demonstrates  
 306 how accuracy could be improved if modeled uncertainty  $\sigma_{ijk}$  decreases.

307 Figure 9 reports the distribution of  $D_a$  (from both the Marshall and Millington-Quirk methods,

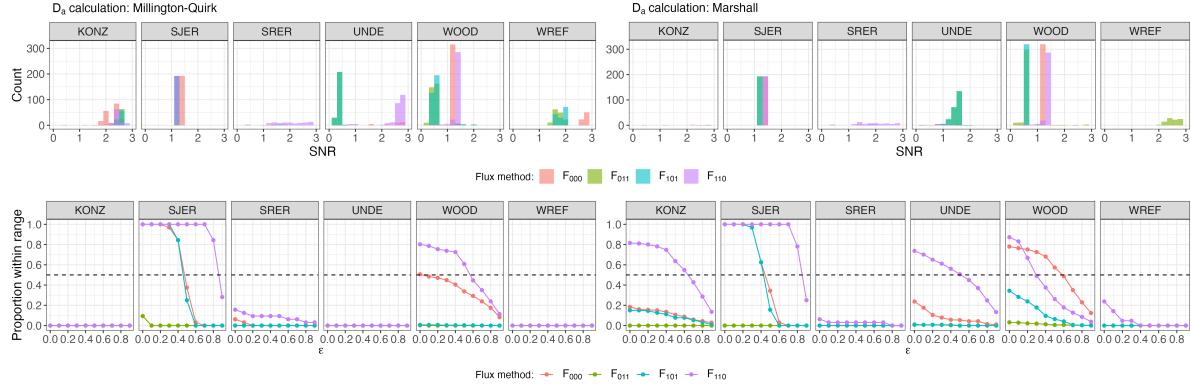


Figure 8: Top panels: distribution of SNR values across each of the different sites for modeled effluxes from the `neonSoilFlux` package, depending on the diffusivity calculation used (Millington-Quirk or Marshall, Section 4.2.2). Bottom panels: Proportion of measured  $F_S$  within the modeled range of a flux computation method  $F_{ijk}$  given an uncertainty reduction factor  $\epsilon$ , or  $|F_S - F_{ijk}| < (1 - \epsilon)\sigma_{ijk}$ .

308 Section 4.2.2) at each study site, and the *post hoc* computation of  $D_a$  (Section 4.2.2).

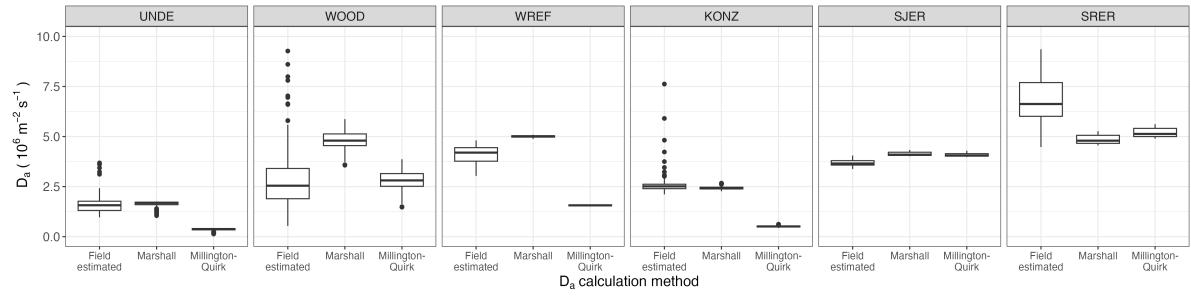


Figure 9

## 309 6 Discussion

310 This study presents a unified data science workflow to efficiently process automated measure-  
 311 ments of belowground soil CO<sub>2</sub> concentrations, water, and temperature to infer estimates of  
 312 soil surface CO<sub>2</sub> effluxes through application of Fick's Law (Equation 4). Our core goals in this  
 313 study were: (1) to generate estimates of soil flux from continuous soil sensor data at terrestrial

314 NEON sites using the flux-gradient method and then (2) to compare those estimates to field-  
315 measured fluxes based on the closed chamber approach at six NEON focal sites. We discuss  
316 our progress toward these core goals through (1) an overall evaluation of the flux-gradient ap-  
317 proach (and uncertainty calculation) and (2) site-specific evaluation of differences in estimated  
318 vs measured fluxes.

319 **6.1 General evaluation of flux-gradient approach**

320 Key assumptions of the flux-gradient approach are that CO<sub>2</sub> concentrations increase through-  
321 out the soil profile. We found that this condition was met at XXX% across the study period.  
322 Periods where this gradient condition are not met generally are connected to biophysical  
323 processes such soil wetting events (e.g. KONZ), which have the effect of reducing the soil res-  
324piration or efflux due to a temporary reduction in diffusivity. When modeling soil respiration,  
325 typically a non-linear response function that also considers soil type is used (Bouma & Bryla,  
326 2000; Yan et al., 2016, 2018). For the `neonSoilFlux` package, soil type is connected to the bulk  
327 density, which was characterized at each NEON site based on replicate samples collected from  
328 the site megapit at a subset of soil horizons, with an estimated uncertainty of ±5% (see NEON  
329 User Guide to Soil physical and chemical properties, Megapit (DP1.00096.001)). Coarse frag-  
330ment estimates also have very large uncertainties, but because the volume fraction tends to  
331 be low in surface soils it probably wouldn't contribute much additional flux uncertainty.

332 The largest source of uncertainty to improve reliability of the flux estimate is to prevent the  
333 usage of gap-filled data. Three sites (KONZ, SRER, and KONZ) had more than 75% of half-  
334 hourly periods with no-gap filled measurements. Two sites (SJER and WOOD) had more  
335 than 75% of half-hourly intervals with just one gap-filled measurement. While WREF re-  
336ported no gap-filled measurements, field data collection occurred following a once-in-a century  
337 rainstorm with soils observed at their water holding capacity. We recommend that whenever

338 available, local field knowledge is supplementary to any QA filtering protocol of fluxes from  
339 the `neonSoilFlux` package.

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

347 Based on this approach, we would *a priori* expect  $F_{011} \leq F_{101} \leq F_{110} \leq F_{000}$  because the  
348 previous flux estimates ones correspond to deeper depths which will could miss CO<sub>2</sub> produced  
349 in shallower layers. Additionally, field flux measurements should correlate with  $F_{000}$  because  
350 they represent surface fluxes.

## 351 **6.2 Evaluation of flux-gradient approach at each site**

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

358 The six sites studied provide separate case studies for considerations when applying the flux-  
359 gradient method to evaluate resulting uncertainties and fluxes For example, SRER is charac-  
360 terized by sandy soil, which also led to the highest observed field soil temperatures. At SRER

361 the flux across the top two layers ( $F_{110}$ ) produced a pattern of soil flux consistent with the ob-  
362 served field data. The remaining methods  $F_{101}$ ,  $F_{011}$ , or  $F_{000}$  are derived from information at  
363 the deeper layer, which is decoupled both in terms of temperature and CO<sub>2</sub> concentration.

364 In addition, KONZ is a site that experienced a significant rain event prior to sampling with  
365 eventual drying out over the course of the experiment. In this case we observed storage of soil  
366 water which increased the soil CO<sub>2</sub> at the top layer, leading to negative values of flux at the  
367 start of the experiment, with the fluxes drying out afterwards. In this case only when the soil  
368 dried out (or returned to a baseline level), that the fluxes at the provided layer would work  
369 out in this case.

370 When considering systematic deployment of this method across a measurement network, we  
371 faced a number of independent challenges for consideration.

372 Figure 8 illustrates the tradeoff between accuracy for modeled fluxes (defined here as closeness  
373 to field-measured  $F_S$ ) and precision defined by the SNR, and how this is confounded by the  
374 choice of diffusivity model used. MORE HERE

375 Diffusivity discussion

376 In developing and validating our approach, we faced a number of challenges related to data  
377 availability, including... gap filling, sensor calibration, depth interpolation, rainstorms, etc  
378 These errors are all

### 379 **6.3 Recommendations for future method development**

380 The `neonSoilFlux` package provides three different approaches of values for a soil flux. We  
381 believe these approaches reflect a variety of site-specific determination and assumptions used  
382 to generate a soil flux measurement (Maier & Schack-Kirchner, 2014), with the choice of

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

386 Figures XXX suggests that the provided uncertainty from `neonSoilFlux` is an overestimate  
387 compared to what is actually computed. When  $\epsilon = 0$  in Figure Figure 8, that means we  
388 are just using the reported uncertainty from `neonSoilFlux`. Looking at that ( $\text{epsilon} = 0$ )  
389 shows field measurements UNDE, KONZ, SJER are 100% within the reported intervals from  
390 `neonSoilFlux`. But those sites tend to have a  $\text{SNR} < 1$ , so the uncertainty is pretty noisy. For  
391 UNDE, we could even reduce the uncertainty by a factor of 75% ( $\text{epsilon} = 0.75$ ), more than  
392 half of the field measurements will still be within the reported intervals. For KONZ, we are  
393 still within 70% of the reported intervals when uncertainty is reduced by 90%. That suggests  
394 that while the reported accuracy (as compared to field measurements), we do have higher  
395 precision.

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

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

407 **7 Conclusions**

- 408 We have here presented an R package `neonSoilFlux` for the estimation of soil CO<sub>2</sub> fluxes from  
409 continuous buried soil sensor measurements across terrestrial National Ecological Observatory  
410 Network sites. We compared the predicted fluxes to those measured directly using a field-based  
411 closed chamber approach. We find that...
- 412 Baldocchi, D. (2014). Measuring fluxes of trace gases and energy between ecosystems and the  
413 atmosphere - the state and future of the eddy covariance method. *Global Change Biology*,  
414 20(12), 3600–3609. <https://doi.org/10.1111/gcb.12649>
- 415 Berenbaum, M. R., Carpenter, S. R., Hampton, S. E., Running, S. W., & Stanzione, D. C.  
416 (2015). *Report from the NSF BIO Advisory Committee Subcommittee on NEON Scope  
417 Impacts*.
- 418 Bond-Lamberty, B. (2018). New Techniques and Data for Understanding the Global Soil Res-  
piration Flux. *Earth's Future*, 6(9), 1176–1180. <https://doi.org/10.1029/2018EF000866>
- 419 Bond-Lamberty, B., Ballantyne, A., Berryman, E., Fluet-Chouinard, E., Jian, J., Morris, K.  
420 A., Rey, A., & Vargas, R. (2024). Twenty Years of Progress, Challenges, and Opportuni-  
421 ties in Measuring and Understanding Soil Respiration. *Journal of Geophysical Research:  
422 Biogeosciences*, 129(2), e2023JG007637. <https://doi.org/10.1029/2023JG007637>
- 423 Bond-Lamberty, B., Christianson, D. S., Malhotra, A., Pennington, S. C., Sihi, D., Aghak-  
424 ouchak, A., Anjileli, H., Altaf Arain, M., Armesto, J. J., Ashraf, S., Ataka, M., Baldocchi,  
425 D., Andrew Black, T., Buchmann, N., Carbone, M. S., Chang, S.-C., Crill, P., Curtis, P.  
426 S., Davidson, E. A., ... Zou, J. (2020). COSORE: A community database for continuous  
427 soil respiration and other soil-atmosphere greenhouse gas flux data. *Global Change Biology*,  
428 26(12), 7268–7283. <https://doi.org/10.1111/gcb.15353>
- 429 Bond-Lamberty, B., & Thomson, A. (2010). A global database of soil respiration data. *Bio-  
430 geosciences*, 7(6), 1915–1926. <https://doi.org/10.5194/bg-7-1915-2010>

- 432 Bond-Lamberty, B., Wang, C., & Gower, S. T. (2004). A global relationship between the  
433 heterotrophic and autotrophic components of soil respiration? *Global Change Biology*,  
434 10(10), 1756–1766. <https://doi.org/10.1111/j.1365-2486.2004.00816.x>
- 435 Bouma, T. J., & Bryla, D. R. (2000). On the assessment of root and soil respiration for soils  
436 of different textures: Interactions with soil moisture contents and soil CO<sub>2</sub> concentrations.  
437 *Plant and Soil*, 227(1), 215–221. <https://doi.org/10.1023/A:1026502414977>
- 438 Chen, H., & Tian, H.-Q. (2005). Does a General Temperature-Dependent Q10 Model of Soil  
439 Respiration Exist at Biome and Global Scale? *Journal of Integrative Plant Biology*, 47(11),  
440 1288–1302. <https://doi.org/10.1111/j.1744-7909.2005.00211.x>
- 441 Davidson, E. A., Janssens, I. A., & Luo, Y. (2006). On the variability of respiration in  
442 terrestrial ecosystems: Moving beyond Q10. *Global Change Biology*, 12, 154–164. <https://doi.org/10.1111/j.1365-2486.2005.01065.x>
- 443 Desai, A. R., Murphy, B. A., Wiesner, S., Thom, J., Butterworth, B. J., Koupaei-Abyazani, N.,  
444 Muttaqin, A., Paleri, S., Talib, A., Turner, J., Mineau, J., Merrelli, A., Stoy, P., & Davis,  
445 K. (2022). Drivers of Decadal Carbon Fluxes Across Temperate Ecosystems. *Journal of  
446 Geophysical Research: Biogeosciences*, 127(12), e2022JG007014. <https://doi.org/10.1029/2022JG007014>
- 447 Elshall, A. S., Ye, M., Pei, Y., Zhang, F., Niu, G.-Y., & Barron-Gafford, G. A. (2018). Relative  
448 model score: A scoring rule for evaluating ensemble simulations with application to micro-  
449 bial soil respiration modeling. *Stochastic Environmental Research and Risk Assessment*,  
450 32(10), 2809–2819. <https://doi.org/10.1007/s00477-018-1592-3>
- 451 Falge, E., Baldocchi, D., Olson, R., Anthoni, P., Aubinet, M., Bernhofer, C., Burba, G.,  
452 Ceulemans, R., Clement, R., Dolman, H., Granier, A., Gross, P., Grünwald, T., Hollinger,  
453 D., Jensen, N.-O., Katul, G., Keronen, P., Kowalski, A., Lai, C. T., ... Wofsy, S. (2001).  
454 Gap filling strategies for defensible annual sums of net ecosystem exchange. *Agricultural  
455 and Forest Meteorology*, 107(1), 43–69. [https://doi.org/10.1016/S0168-1923\(00\)00225-2](https://doi.org/10.1016/S0168-1923(00)00225-2)

- 458 Farrance, I., & Frenkel, R. (2012). *Uncertainty of Measurement: A Review of the Rules*  
459 *for Calculating Uncertainty Components through Functional Relationships.* *The Clinical*  
460 *Biochemist Reviews*, 33(2), 49–75.
- 461 Friedlingstein, P., O’Sullivan, M., Jones, M. W., Andrew, R. M., Bakker, D. C. E., Hauck,  
462 J., Landschützer, P., Le Quéré, C., Luijkx, I. T., Peters, G. P., Peters, W., Pongratz, J.,  
463 Schwingshackl, C., Sitch, S., Canadell, J. G., Ciais, P., Jackson, R. B., Alin, S. R., Anthoni,  
464 P., ... Zheng, B. (2023). Global Carbon Budget 2023. *Earth System Science Data*, 15(12),  
465 5301–5369. <https://doi.org/10.5194/essd-15-5301-2023>
- 466 Hamdi, S., Moyano, F., Sall, S., Bernoux, M., & Chevallier, T. (2013). Synthesis analysis  
467 of the temperature sensitivity of soil respiration from laboratory studies in relation to  
468 incubation methods and soil conditions. *Soil Biology and Biochemistry*, 58, 115–126. <https://doi.org/10.1016/j.soilbio.2012.11.012>
- 470 Hirano, T., Kim, H., & Tanaka, Y. (2003). Long-term half-hourly measurement of soil CO<sub>2</sub>  
471 concentration and soil respiration in a temperate deciduous forest. *Journal of Geophysical*  
472 *Research: Atmospheres*, 108(D20). <https://doi.org/10.1029/2003JD003766>
- 473 Jackson, R. B., Lajtha, K., Crow, S. E., Hugelius, G., Kramer, M. G., & Piñeiro, G. (2017).  
474 The Ecology of Soil Carbon: Pools, Vulnerabilities, and Biotic and Abiotic Controls.  
475 *Annual Review of Ecology, Evolution and Systematics*, 48(Volume 48, 2017), 419–445.  
476 <https://doi.org/10.1146/annurev-ecolsys-112414-054234>
- 477 Jian, J., Bailey, V., Dorheim, K., Konings, A. G., Hao, D., Shiklomanov, A. N., Snyder, A.,  
478 Steele, M., Teramoto, M., Vargas, R., & Bond-Lamberty, B. (2022). Historically inconsis-  
479 tent productivity and respiration fluxes in the global terrestrial carbon cycle. *Nature*  
480 *Communications*, 13(1), 1733. <https://doi.org/10.1038/s41467-022-29391-5>
- 481 Jian, J., Vargas, R., Anderson-Teixeira, K., Stell, E., Herrmann, V., Horn, M., Kholod, N.,  
482 Manzon, J., Marchesi, R., Paredes, D., & Bond-Lamberty, B. (2021). A restructured and  
483 updated global soil respiration database (SRDB-V5). *Earth System Science Data*, 13(2),

- 484 255–267. <https://doi.org/10.5194/essd-13-255-2021>
- 485 Jiang, J., Feng, L., Hu, J., Liu, H., Zhu, C., Chen, B., & Chen, T. (2024). Global soil  
486 respiration predictions with associated uncertainties from different spatio-temporal data  
487 subsets. *Ecological Informatics*, 82, 102777. <https://doi.org/10.1016/j.ecoinf.2024.102777>
- 488 Jobbág, E. G., & Jackson, R. B. (2000). The Vertical Distribution of Soil Organic Carbon  
489 and its Relation to Climate and Vegetation. *Ecological Applications*, 10(2), 423–436. [https://doi.org/10.1890/1051-0761\(2000\)010%5B0423:TVDOSO%5D2.0.CO;2](https://doi.org/10.1890/1051-0761(2000)010%5B0423:TVDOSO%5D2.0.CO;2)
- 490 Liu, K., Li, X., Wang, S., & Zhang, H. (2023). A robust gap-filling approach for European  
491 Space Agency Climate Change Initiative (ESA CCI) soil moisture integrating satellite  
492 observations, model-driven knowledge, and spatiotemporal machine learning. *Hydrology  
493 and Earth System Sciences*, 27(2), 577–598. <https://doi.org/10.5194/hess-27-577-2023>
- 494 Luo, Y., Ogle, K., Tucker, C., Fei, S., Gao, C., LaDeau, S., Clark, J. S., & Schimel, D. S. (2011).  
495 Ecological forecasting and data assimilation in a data-rich era. *Ecological Applications*,  
496 21(5), 1429–1442. <https://doi.org/10.1890/09-1275.1>
- 497 Maier, M., & Schack-Kirchner, H. (2014). Using the gradient method to determine soil gas  
498 flux: A review. *Agricultural and Forest Meteorology*, 192–193, 78–95. <https://doi.org/10.1016/j.agrformet.2014.03.006>
- 500 Mariethoz, G., Linde, N., Jougnot, D., & Rezaee, H. (2015). Feature-preserving interpolation  
501 and filtering of environmental time series. *Environmental Modelling & Software*, 72, 71–76.  
502 <https://doi.org/10.1016/j.envsoft.2015.07.001>
- 503 Marshall, T. J. (1959). The Diffusion of Gases Through Porous Media. *Journal of Soil Science*,  
504 10(1), 79–82. <https://doi.org/10.1111/j.1365-2389.1959.tb00667.x>
- 505 Millington, R. J., & Shearer, R. C. (1971). Diffusion in aggregated porous media. *Soil Science*,  
506 111(6), 372–378.
- 507 Moffat, A. M., Papale, D., Reichstein, M., Hollinger, D. Y., Richardson, A. D., Barr, A. G.,  
508 Beckstein, C., Braswell, B. H., Churkina, G., Desai, A. R., Falge, E., Gove, J. H., Heimann,

- 510 M., Hui, D., Jarvis, A. J., Kattge, J., Noormets, A., & Stauch, V. J. (2007). Comprehensive  
511 comparison of gap-filling techniques for eddy covariance net carbon fluxes. *Agricultural and*  
512 *Forest Meteorology*, 147(3), 209–232. <https://doi.org/10.1016/j.agrformet.2007.08.011>
- 513 Moldrup, P., Olesen, T., Yamaguchi, T., Schjønning, P., & Rolston, D. E. (1999). Modeling  
514 diffusion and reaction in soils: 9. The Buckingham-Burdine-Campbell equation for gas  
515 diffusivity in undisturbed soil. *Soil Science*, 164(2), 75.
- 516 National Ecological Observatory Network (NEON). (2024a). *Barometric pressure*  
517 (*DP1.00004.001*). National Ecological Observatory Network (NEON). <https://doi.org/10.48443/RT4V-KZ04>
- 519 National Ecological Observatory Network (NEON). (2024b). *Soil CO<sub>2</sub> concentration*  
520 (*DP1.00095.001*). National Ecological Observatory Network (NEON). <https://doi.org/10.48443/E7GR-6G94>
- 522 National Ecological Observatory Network (NEON). (2024c). *Soil physical and chemical properties*, *Megapit* (*DP1.00096.001*). National Ecological Observatory Network (NEON). <https://doi.org/10.48443/S6ND-Q840>
- 525 National Ecological Observatory Network (NEON). (2024d). *Soil temperature* (*DP1.00041.001*).  
526 National Ecological Observatory Network (NEON). <https://doi.org/10.48443/Q24X-PW21>
- 527 National Ecological Observatory Network (NEON). (2024e). *Soil water content and water*  
528 *salinity* (*DP1.00094.001*). National Ecological Observatory Network (NEON). <https://doi.org/10.48443/A8VY-Y813>
- 530 Norman, J. M., Kucharik, C. J., Gower, S. T., Baldocchi, D. D., Crill, P. M., Rayment, M.,  
531 Savage, K., & Striegl, R. G. (1997). A comparison of six methods for measuring soil-  
532 surface carbon dioxide fluxes. *Journal of Geophysical Research: Atmospheres*, 102(D24),  
533 28771–28777. <https://doi.org/10.1029/97JD01440>
- 534 Phillips, C. L., Bond-Lamberty, B., Desai, A. R., Lavoie, M., Risk, D., Tang, J., Todd-Brown,  
535 K., & Vargas, R. (2017). The value of soil respiration measurements for interpreting and

- 536 modeling terrestrial carbon cycling. *Plant and Soil*, 413(1), 1–25. <https://doi.org/10.1007/s11104-016-3084-x>
- 537
- 538 Raftery, A. E., Gneiting, T., Balabdaoui, F., & Polakowski, M. (2005). *Using Bayesian Model*  
539 *Averaging to Calibrate Forecast Ensembles*. <https://doi.org/10.1175/MWR2906.1>
- 540 Sallam, A., Jury, W. A., & Letey, J. (1984). Measurement of Gas Diffusion Coefficient under  
541 Relatively Low Air-filled Porosity. *Soil Science Society of America Journal*, 48(1), 3–6.  
542 <https://doi.org/10.2136/sssaj1984.03615995004800010001x>
- 543 Shao, J., Zhou, X., Luo, Y., Li, B., Aurela, M., Billesbach, D., Blanken, P. D., Bracho, R.,  
544 Chen, J., Fischer, M., Fu, Y., Gu, L., Han, S., He, Y., Kolb, T., Li, Y., Nagy, Z., Niu, S.,  
545 Oechel, W. C., ... Zhang, J. (2015). Biotic and climatic controls on interannual variability  
546 in carbon fluxes across terrestrial ecosystems. *Agricultural and Forest Meteorology*, 205,  
547 11–22. <https://doi.org/10.1016/j.agrformet.2015.02.007>
- 548 Shao, P., Zeng, X., Moore, D. J. P., & Zeng, X. (2013). Soil microbial respiration from  
549 observations and Earth System Models. *Environmental Research Letters*, 8(3), 034034.  
550 <https://doi.org/10.1088/1748-9326/8/3/034034>
- 551 Sih, D., Gerber, S., Inglett, P. W., & Inglett, K. S. (2016). Comparing models of microbial–  
552 substrate interactions and their response to warming. *Biogeosciences*, 13(6), 1733–1752.  
553 <https://doi.org/10.5194/bg-13-1733-2016>
- 554 Tang, J., Baldocchi, D. D., Qi, Y., & Xu, L. (2003). Assessing soil CO<sub>2</sub> efflux using continuous  
555 measurements of CO<sub>2</sub> profiles in soils with small solid-state sensors. *Agricultural and Forest*  
556 *Meteorology*, 118(3), 207–220. [https://doi.org/10.1016/S0168-1923\(03\)00112-6](https://doi.org/10.1016/S0168-1923(03)00112-6)
- 557 Tang, J., Misson, L., Gershenson, A., Cheng, W., & Goldstein, A. H. (2005). Continuous  
558 measurements of soil respiration with and without roots in a ponderosa pine plantation  
559 in the Sierra Nevada Mountains. *Agricultural and Forest Meteorology*, 132(3), 212–227.  
560 <https://doi.org/10.1016/j.agrformet.2005.07.011>
- 561 Taylor, J. R. (2022). *An Introduction to Error Analysis: The Study of Uncertainties in Physical*

- 562      *Measurements, Third Edition* (3rd ed.). University Science Press.
- 563      Yan, Z., Bond-Lamberty, B., Todd-Brown, K. E., Bailey, V. L., Li, S., Liu, C., & Liu, C. (2018).
- 564      A moisture function of soil heterotrophic respiration that incorporates microscale processes.
- 565      *Nature Communications*, 9(1), 2562. <https://doi.org/10.1038/s41467-018-04971-6>
- 566      Yan, Z., Liu, C., Todd-Brown, K. E., Liu, Y., Bond-Lamberty, B., & Bailey, V. L. (2016).
- 567      Pore-scale investigation on the response of heterotrophic respiration to moisture conditions
- 568      in heterogeneous soils. *Biogeochemistry*, 131(1), 121–134. <https://doi.org/10.1007/s10533-016-0270-0>
- 570      Zhang, R., Kim, S., Kim, H., Fang, B., Sharma, A., & Lakshmi, V. (2023). Temporal
- 571      Gap-Filling of 12-Hourly SMAP Soil Moisture Over the CONUS Using Water Balance
- 572      Budgeting. *Water Resources Research*, 59(12), e2023WR034457. <https://doi.org/10.1029/2023WR034457>