

The eddy-covariance storage term in air: Consistent community resources improve flux measurement reliability



Ke Xu^{a,b,*}, Natchaya Pingintha-Durden^a, Hongyan Luo^a, David Durden^a, Cove Sturtevant^a, Ankur R. Desai^b, Christopher Florian^a, Stefan Metzger^{a,b}

^a National Ecological Observatory Network, Battelle, 1685 38th Street, Boulder, CO 80301, USA

^b University of Wisconsin-Madison, Department of Atmospheric and Oceanic Sciences, 1225 West Dayton Street, Madison, WI 53706, USA

^c University of Michigan-Ann Arbor, Climate and Space Sciences and Engineering, 2455 Hayward Street, Ann Arbor, MI 48109, USA

ARTICLE INFO

Keywords:

Eddy covariance
Air storage term
National Ecological Observatory Network
Greenhouse gases

ABSTRACT

In the widely-used eddy-covariance (EC) technique, it is often assumed that the air storage term, i.e. the change of below-turbulence-sensor scalar abundance, is negligible or comprises a small part of net surface-atmosphere exchange (NSAE). Previous studies have demonstrated that this assumption is often violated where non-turbulent processes prevail, and thus it is important to measure and calculate air storage in flux measurements. However, the implementation of air storage measurement and calculation is not ubiquitous as EC standard turbulent flux. In most cases, air storage is not a standard data product or even neglected in EC flux tower measurements. In other cases, air storage term is calculated simply using only the measurements at the tower top. This gap between the ideal initiative and actual implementation motivates us to derive and release one of the first community resources to facilitate the consistent measurement and calculation of EC air storage across sites. These resources include (i) the standardized air storage term measurement setup design at National Ecological Observatory Network (NEON) sites; (ii) the development and public release of the eddy4R.stor open-source air storage R-package; (iii) the derivation and public release of storage term data products, measured and calculated consistently across 47 NEON sites; and (iv) exploration the scientific usefulness of these resources through example use cases, specifically the exploration of the bias of the air storage term when different measurement level intensity used and exploration of the air storage term pattern. We expect the consistent air storage measurement and calculation can better serve the overall purpose of the EC technique to provide more reliable measurement of NSAE for the community. This can further benefit the community accurate depiction of the sub-daily to diurnal cycle of surface fluxes in doing carbon cycle flux partitioning, land modeling, and studying ecosystem response to weather extremes.

1. Introduction

For decades, the eddy-covariance (EC) technique has been used extensively to measure net surface-atmosphere exchange (NSAE) at hundreds of sites across the globe. EC observations, such as those collected by AmeriFlux and the National Ecological Observatory Network (NEON), have become available at unprecedented temporal duration and distributed spatial extents (Novick et al., 2018). The longest running towers are now approaching three decades of observations (Baldocchi, 2008). This makes EC one of the most important techniques to sample surface fluxes at regional scale for studying land-atmosphere interactions, e.g. detection of localized CO₂ sources (Schwandner et al., 2017), ecosystem sensitivity to temperature, dryness, and change of

phenology (Wolf et al., 2017; Desai, 2014; Mahecha et al., 2017; Tang et al., 2014).

One key underlying principle of EC measurements from a tower is Taylor Hypothesis, which assumes the eddies do not change substantially during the time period they are passing by the tower (Taylor, 1938). Using numerous assumptions (discussed below), it is possible to set the tower-measured half-hourly/hourly turbulent flux, i.e. the covariance of vertical wind speed and the scalar of interest, equal to the net surface-atmosphere exchange.

Central to this simplification is the steady state assumption, which by virtue of time-space aggregation requires both, temporal stationarity and spatial homogeneity. Temporal stationarity that air storage, term I in Eq. (1), is negligible or comprises a small part of NSAE, provided

* Corresponding author at: Department of Atmospheric and Oceanic Sciences, University of Wisconsin-Madison, 1225 W. Dayton Street, Madison, WI 53706, USA.
E-mail address: kxu35@wisc.edu (K. Xu).

sufficient turbulence (Foken and Wichura, 1996; Massman and Lee, 2002). Spatial homogeneity implies that either all observations represent the same, fixed control volume, or different, time-varying control volumes over a horizontally uniform surface (e.g., Raupach, 1988; Foken and Wichura, 1996). In the following we focus on the temporal stationarity aspect (term I in Eq. (1)), and address spatial homogeneity elsewhere (Metzger, 2018; Xu et al., 2017).

$$NSAE = \int_0^{d_{z,m}} \frac{\partial \bar{X}}{\partial t} dz + \int_0^{d_{z,m}} \frac{\partial \bar{w'X'}}{\partial z} dz \quad (1)$$

where X is a scalar quantity; w is vertical wind speed; t is time, and $d_{z,m}$ is the measurement height. The overbars indicate a time average and primes ($'$) denote turbulent fluctuations. Term II is the vertical turbulent flux. Term I in Eq. (1) is the vertically integrated change of below-sensor scalar abundance, equivalent to the storage term.

Although storage term is often assumed to average to zero on daily and longer time scales, this assumption is hypothesized to be violated where non-turbulent processes prevail, such as in the nighttime stable boundary layer (Aubinet et al., 2005; 2008; 2012; van Gorsel et al., 2009), over complex terrain (Monson et al., 2005), in tall canopies (Massman and Lee, 2002), at tall tower sites (Desai et al., 2014), as well as during transition times (van Gorsel et al., 2007).

In most cases, in order to limit the influence of large air storage terms, flux observations are often filtered for periods that fulfill these conditions as a practical workaround in standard EC processing, such as widely-used steady-state tests and u^* -filtering (Foken, 2008; Janssens et al., 2001; Zhao et al., 2006; Aubinet, 2008). As a result, fewer occurrences of large air storage terms remain in the filtered time series. Most times, the data gaps created by the filtering require imputation (Falge et al., 2001; Papale and Valentini, 2003; Juang et al., 2006) introduces a new source of uncertainty. This data filtering and filling can result in an inaccurate depiction of NSAE and energy, water, and carbon diurnal patterns. For example, neglection of air storage term has also been shown to lead flux partitioning methods to overestimate photosynthesis (Aubinet, 2008). Although Foken (2008) stated that air storage term is not sufficient to explain observed energy budget imbalances, recent studies showed that accounting for air storage terms along with soil and vegetation storage terms improve energy balance closure especially at short time scales (Lindroth et al., 2010; Leuning et al., 2012; Burns et al., 2015; Swenson et al., 2019; Reed et al., 2018; Xu et al., 2017; Eshonkulov et al., 2019).

Although some previous works demonstrated the importance of air storage term in net ecosystem exchange and gave general guidance about EC air storage term measurement (e.g. Aubinet et al., 2012), the implementation of consistent air storage term measurement and calculation is not ubiquitous at all. In most cases, air storage term is not a standard data product or even neglected in EC flux tower measurements. In other cases, air storage term is calculated using only the measurements at the tower top (Nicolini et al., 2018). The gap between the ideal initiative and actual implementation mainly lies in i) the limited resources of the measurement system; and ii) the lack of the guidance about the explicit operational set up, algorithmic calculation, and release of standard calculation software. These situations imply that more efforts are needed to i) provide explicit measurement and calculation guidance as well as easily assessible software for the community to consistently investigate the EC air storage term; and ii) to show the importance of storage term data products being similarly measured and derived across sites. Hence, our goal of this manuscript is to narrow the gap by deriving and releasing one of the first community air storage term resources. These resources include:

- (i) the standardized storage term measurement setup at National Ecological Observatory Network (NEON) sites (Section 2.1);
- (ii) the development and public release of the eddy4R.stor open-source

- storage term R-package (Sections 2.2–2.3);
- (iii) the derivation and public release of NEON storage term data products, measured and calculated consistently across 47 NEON sites (Section 2.4); and
- (iv) exploration the scientific usefulness of these resources through example use cases (Section 3), specifically exploration of the bias of the air storage term when different measurement level intensity used and exploration of the air storage term pattern.

We expect these resources can facilitate the consistent measurement and calculation of EC air storage term across sites and can better serve the overall purpose of the eddy-covariance technique to provide more reliable measurement of NSAE for the community. This can further benefit the community to do better carbon flux partitioning and to better understand the global carbon cycle and the ecosystem response to extreme weather.

2. Air storage term measurements, processing, and data products

First, we introduce the instruments for the vertical profile measurements used in this study, followed by the eddy4R.stor package, including specific algorithmic implementation details, and finally the NEON EC storage term data products.

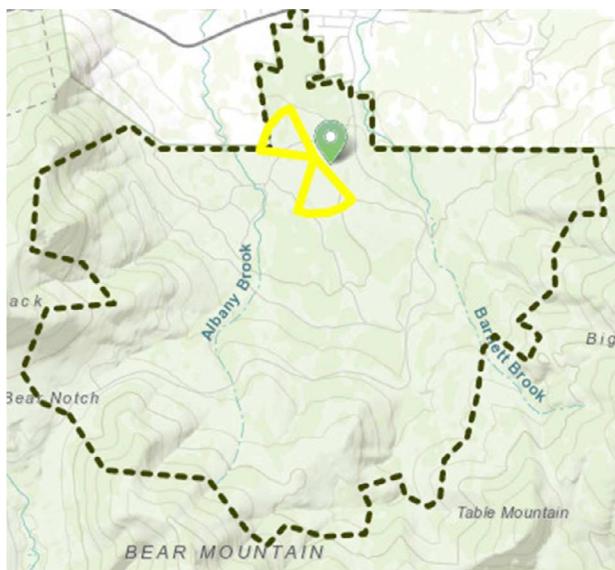
2.1. Measurements

At all NEON sites an Infrared Gas Analyzer (IRGA) (LI-840A; LI-COR Biosciences, Lincoln, NE) is housed in a climate-controlled instrument hut. The IRGA reports CO_2 and H_2O concentrations at a frequency of 1 Hz, while switching between different vertical tower measurement levels. At each measurement level, the IRGA measures CO_2 and H_2O for about 180 s, of which only the last 120 s are used for calculation to avoid the memory effects from the previous level (Andrews et al., 2014). This 180 s sampling time and 120 s processing per measurement level were set by the WMO recommendation of 0.1 ppm precision for CO_2 (WMO, 2014) and Allan variance test results for LI840A sensor conducted at NEON Headquarters (Andrew et al., 2014). For measurement time shorter than these, the variance is too high to achieve the required 0.1 ppm precision. Such a strategy implies that the revisit time for measuring a given vertical level increases with the total number of vertical levels. As a result, vertical spatial resolution of the gas concentration measurements is traded off against their temporal resolution. At most NEON sites, given that the measurement time at a single vertical level is about 180 s, the period of time for a sensor to switch through a set of total four to six measurement levels is about 720–1080 s. In Section 3.2, as an example scientific application case using three field sites, we found that all levels, i.e. five or six levels at three sites, are necessary to estimate storage term accurately and precisely.

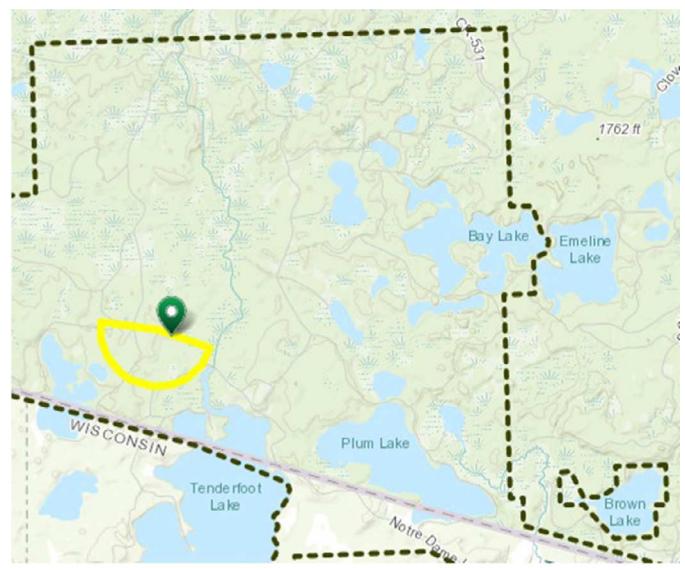
The storage of heat is calculated from the temperature profile measurements using PRT sensors (R032-00000048, Thermometrics Cooperation, Northridge, CA), which measure air temperature continuously at each level at 1 Hz. In Section 2.2, we calculate the EC storage term using the eddy4R.stor package with vertical profile measurement levels.

2.2. The eddy4R.stor package

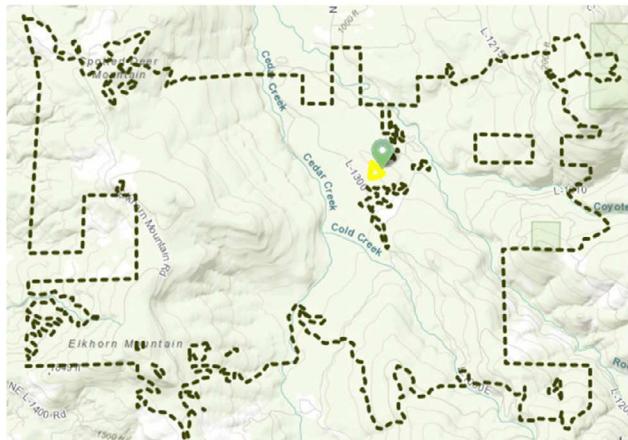
The eddy4R.stor package is one of a suite of eddy4R family for EC data processing, and modularly expands on the work presented in Metzger et al. (2017): the eddy4R family is built upon a development and systems operation approach (DevOps), which produces reproducible, open-source, and extensible software, released and iterated by the Git version control system. Controlled terminology is used as a configuration tool for sustainable community collaboration and continued development. Here, we make the eddy4R.stor package publicly



a) BART



b) UNDE



c) ABBY

Fig. 1. Overview maps of BART, UNDERC, and ABBY tower sites and surrounding areas. Source: <https://www.neonscience.org/field-sites/field-sites-map>.

Table 1

Basic information of BART, UNDE, and ABBY sites.

Site name	BART	UNDE	ABBY
Tower height [m]	36	39	19
Lat, Lon [$^{\circ}$ N, $^{\circ}$ E]	44.06388, -71.28731	46.23388, -89.53725	45.76243, -122.33033
Canopy height [m]	20	23	4
Tower Levels	6 (3 within canopy)	6 (3 within canopy)	5 (2 within canopy)
Ecosystem	Deciduous Forest: maple and beech	Both deciduous and evergreen forests, affected by terrain	Conifer forest, Reforested forest, roads, logging, young forest
Climate classification	Warm summer, humid continental climate	Warm summer humid continental climate	Temperate Mediterranean climate
Surface heterogeneity	relatively homogeneous	relatively heterogeneous	relatively heterogeneous
Link to comprehensive site description	https://www.neonscience.org/field-sites/field-sites-map/BART	https://www.neonscience.org/field-sites/field-sites-map/UNDE	https://www.neonscience.org/field-sites/field-sites-map/ABBY
Data coverage	49%	89%	35%

available with the source code housed in a version-controlled repository (The link will be here when the manuscript published). Previous to this release, eddy4R.base and eddy4R.qaqc have already been published; some functions and wrappers in the prior two packages are used in eddy4R.stor, e.g. reading in data, quality assessment and quality control. NSAE is produced as a standard NEON data product by combining

the products of the eddy4R.stor package with those from the eddy4R.turb package, which calculates turbulent flux.

2.3. Algorithm theory

Described below is the theory of eddy4R.stor algorithms used to

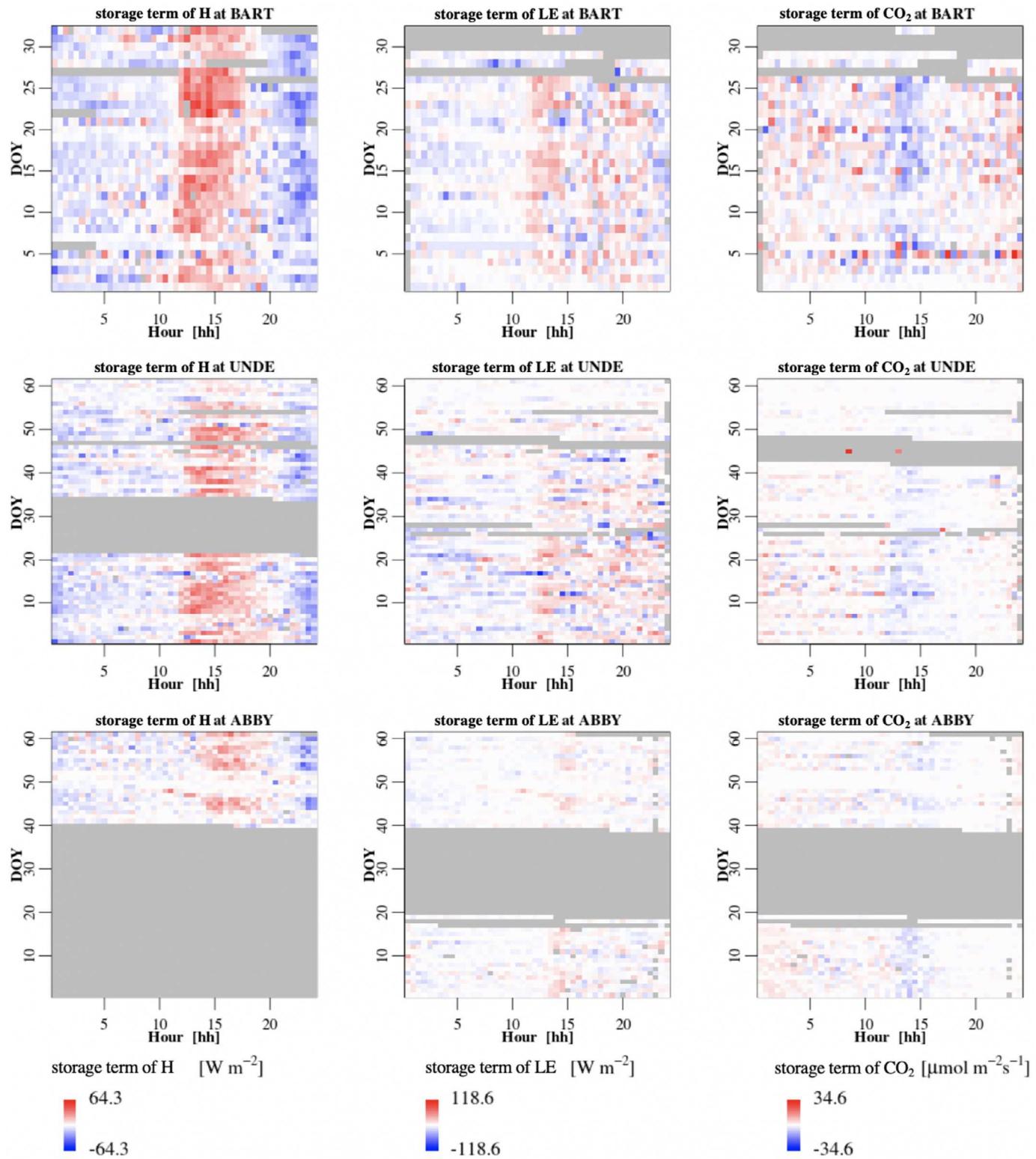


Fig. 2. Fingerprint plots of EC storage term of H, LE, and CO_2 (columns) for BART, UNDE, and ABBY sites (rows). Grey areas are missing data.

process the CO_2 , H_2O mixing ratios, and temperature in the atmosphere, as well as the mathematical derivation of the storage term. The first step is to apply de-spiking to all time series signals collected for the eddy covariance storage exchange (ECSE) assembly (Brock, 1986; Starkenburg et al., 2016). Then the mean, variance and standard error of atmospheric temperature, CO_2 and H_2O concentrations are calculated for the effective measurement time, ~ 120 s. These are stored as

the ECSE assembly level 1 data product (dp01). The computation for NEON EC storage term data products of CO_2 , H_2O , and temperature then follows the steps of temporal interpolation, calculating time rate of change (level 2 data product, dp02), vertical interpolation (level 3 data product, dp03), and vertical integration of EC storage term (level 4 data product, dp04).

The ECSE level 2 data products are defined as the time rate of

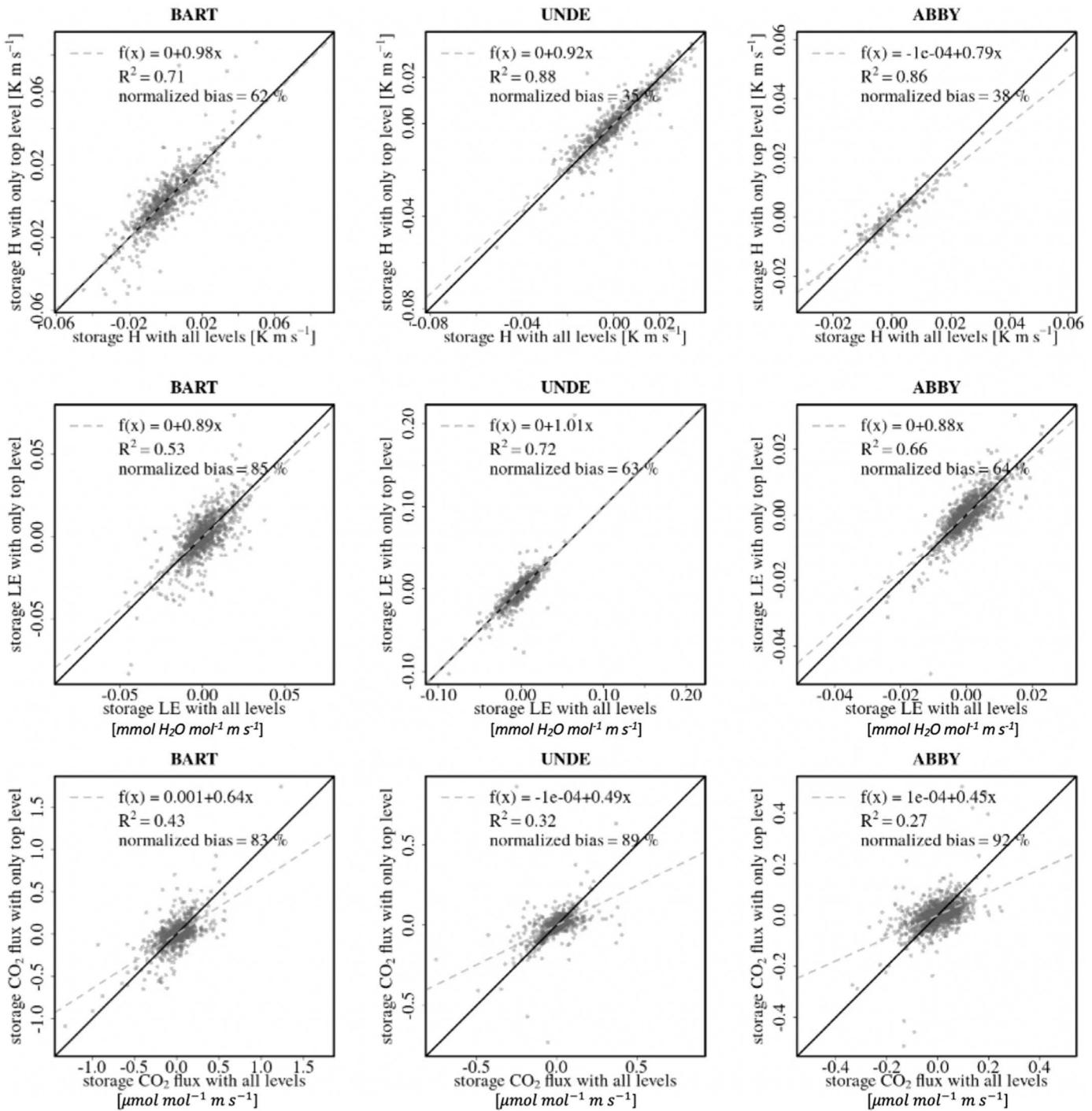


Fig. 3. Comparison of EC storage terms of H, LE and CO₂ (three rows) calculated with all levels and only top level measurements at BART, UNDE, and ABBY, shown as three columns.

change of scalars. For this purpose, the mean of temperature, CO₂, and H₂O in ECSE level 1 data products are first linearly interpolated at 1 min resolution. Both the interpolation method and resolved temporal resolution can be adjusted for different locations and in different applications. The ECSE level 2 data products are then calculated from the four-minute time average at the end of a half hour, minus the four-minute time average at the beginning of the same half hour (Eq. (2)). For example, assuming that air storage term estimates are to be computed for timestamp 07:30:00, then by convention the 07:30:00 timestamp represents the storage term corresponding to observations between 07:30:00 and 08:00:00. dX, where X stands for each scalar, will

then be computed from the time average of measurements from 07:58:00 to 08:02:00 minus the time average of measurements from 07:28:00 to 07:32:00,

$$\frac{dX}{dt} = \frac{\bar{X}_{t \geq t_b - 2 \text{ min and } t < t_e + 2 \text{ min}} - \bar{X}_{t \geq t_b - 2 \text{ min and } t < t_b + 2 \text{ min}}}{30 \text{ min}} \quad (2)$$

where t_b is the beginning time of the first minute in the 30 min block, and t_e is the last minute of the 30 min block. In terms of integral window size, we should avoid that EC storage term estimates be influenced by single eddies penetrating inside the canopy, and we should use for the EC storage term computation a period long enough to capture an adequate number (~10) of these eddies to avoid introducing

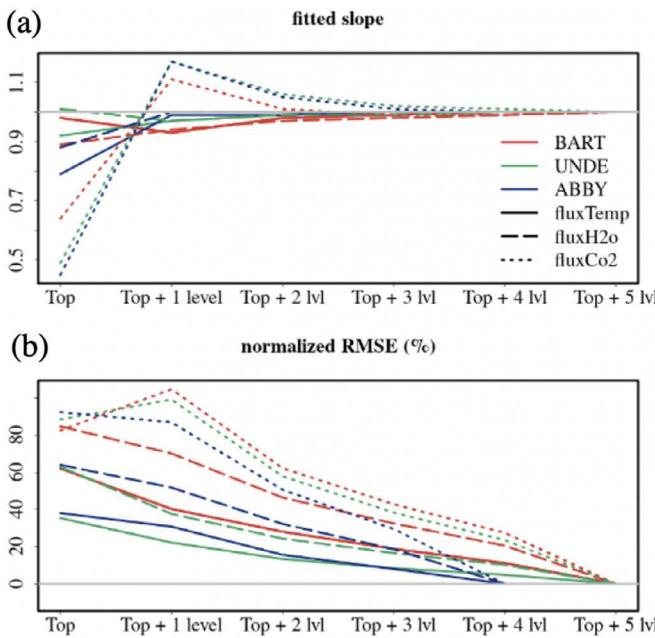


Fig. 4. The fitted slope (subplot a) and normalized RMSE (subplot b) between reference EC storage term with all level measurements and estimated storage term with i) only top level and ii) top level measurements as well as randomly chosen one to all levels below the top level. (abbreviated as “lvl” in the x axis label).

bias to the profiles or single observational points. Finnigan (2006) and Montagnani et al. (2018) suggested the use of time averaged window size from 180 to 300 s depending on the degree of turbulence development and site condition, with the longer integration time for less turbulent conditions as observed in taller canopies. Given the wide differences in the turbulent characteristics existing at the NEON ecosystem stations, we choose 240 s as default value with flexibility to be adjusted for different locations and in applications. The temporal resolution of ECSE dp02 is set to be 30 min for combination with EC turbulent exchange (ECTE) data products.

ECSE dp03 is the vertically resolved time rate of change based on ECSE dp02. The default interpolation method is trapezium interpolation, and the default vertical resolution is 0.1 m. Both the interpolation method and vertical resolution can be adjusted for different locations and different applications. 0.1 m vertical resolution is chosen because NEON measurement levels are accurate to one decimal place by default. Coarser than 0.1 m interpolated resolution will blur the position where the time rate of change is measured. The higher than 0.1 m resolution can be applied, but the ECSE dp04 storage term will not change even with higher resolution, since ECSE dp04 is the integral of the linear interpolated dp03 as shown below.

The ECSE dp04 EC storage term is then integrated from dp03, time rate of change vertical profiles:

$$\text{fluxStor}(X) = \int_0^{\max(\text{DistZaxsLvlMeasTow})} \frac{dX}{dt} dz \quad (3)$$

where fluxStor is EC storage term, X is a scalar quantity such as H_2O or CO_2 mixing ratios, and $\text{DistZaxsLvlMeasTow}$ represents profile measurement heights. This EC storage term is part of the NEON NSAE dp04 data products.

Integrated Carbon Observation System (ICOS, Montagnani et al., 2018) and eddyPro (LI-COR, Inc. Lincoln, USA) use similar algorithm to determine EC storage term as eddy4R.stor, except for some subtle settings, e.g. different sampling time. Similar algorithms make the EC storage term data products produced by these algorithms interoperable. Further comparisons can be done to fully explore the difference between different algorithm implementations.

2.4. NEON air storage term data products

The NEON Data Portal (<http://data.neonscience.org/home>) hosts all NEON-generated data products. All data products are thoroughly described in the NEON Data Product catalog (<http://data.neonscience.org/data-product-catalog>), and during data download users may choose to include all relevant documentation for the data product, which may also be explored separately in the NEON Document Library (<http://data.neonscience.org/documents>). For programmatic retrieval of NEON data, users may utilize the NEON application programming interface (<http://data.neonscience.org/data-api>) to directly pull data from the NEON database.

ECSE data are provided in NEON standard Hierarchical Data Format Version 5 (HDF5) files. The capability of is reliant upon efficient input or output of data, data compressibility to reduce compute resource loads, and the ability to easily package and access metadata. Each ECSE file comprises Level 1–Level 4 data products generated from the algorithm described in Section 2.3. L1 data products include the profile of temperature, CO_2 concentration, H_2O concentration at each measurement level and corresponding validation data. ECSE L2 data products are the time rate of change of temperature, CO_2 concentration, H_2O concentration at each half hour. ECSE L3 data products are the vertically resolved time rate of change at each half hour based on ECSE dp02. ECSE L4 is the EC storage term, which is integrated from vertical profiles of time rate of change (L3). ECSE storage HDF 5 data are ready at the NEON Data Portal for NEON sites in a near-real-time pipeline, i.e. data product available within 30 days from data acquisition.

3. Example applications

In the following, we present two example applications to test scientific usefulness of the air storage term resources that we developed and released above (in Section 2). Specifically, we applied the resources to explore how large the uncertainty of air storage term is when different level intensity are used (Section 3.2) and to explore EC storage term pattern (Section 3.3) at three sites (Section 3.1), with code development, packaging, release, and operation about the NEON air storage term presented in this paper.

3.1. Sites

We chose NEON EC sites for this study, because NEON provides standardized observations and data processing designed specifically for inter-site comparability and analysis (Metzger et al., 2019). NEON data, software, and services have now become available at the NEON Data Portal and github public repository (Metzger et al., 2017). From the Data Portal, we chose three sites, Bartlett Experimental Forest (BART), University of Notre Dame Environmental Research Center (UNDE), and Abby Road (ABBY) as shown in Fig. 1. These three sites cover a variety of different kinds of forests, different tower heights, different kinds of homogeneity and different canopy heights. BART is a relatively homogeneous canopy (within the flux footprint) eastern deciduous forest dominated by maple and beech. The BART tower (36 m) has 6 levels, and canopy height is about 20 m. UNDE consists of heterogeneous mixed forests, wetlands, and lakes in the central US, with a canopy height of about 23 m. The UNDE tower has 6 measurement levels along its 39 m height. ABBY is a young, heterogeneous, reforested coniferous forest in the western US, with a canopy height of 4 m. Its 19 m tower has 5 levels. Basic information about these sites is listed in Table 1. We used 2017 September and October data, when the ecosystem transitions from greenness to senescence with temporally varying surface and meteorological forcings. The three sites offer spatial and temporal variability and different magnitudes of energy/carbon budgets and EC storage terms. To give an overview of the data that we used in this manuscript, finger-print plots are made for storage H, LE, and CO_2 flux over all three sites (Fig. 2).

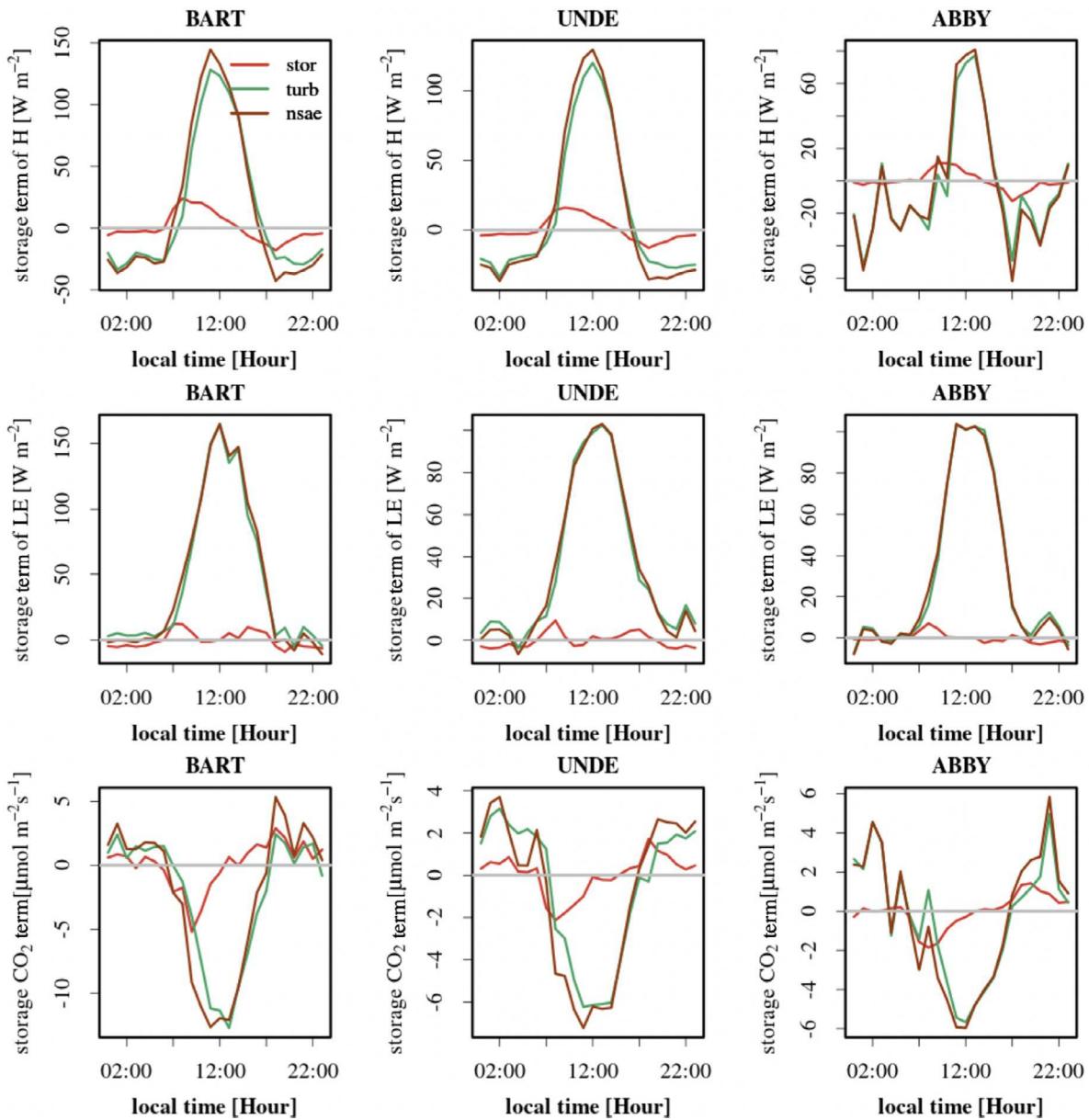


Fig. 5. Mean diurnal cycle of storage (stor) and turbulent flux (turb), and net surface-atmosphere exchange (nsae) of H, LE, and CO₂ (columns) for BART, UNDE, and ABBY sites (rows).

3.2. Test the uncertainty of air storage term when using different vertical profile levels

This test is to explore how large the bias of air storage term is when different measurement level intensity is used and to test how many vertical profile levels are sufficient to accurately estimate EC storage term. We first compared a special case of only using tower top concentration to the EC storage term calculated with all levels at three sites, ABBY, BART, and UNDE. We then computed the fitted linear regression, R^2 , and root mean square deviation (RMSE) between the two methods. Normalized RMSE is calculated as the RMSE normalized by the standard deviation of the EC storage term computed with all levels:

$$RMSE = \sqrt{\frac{1}{N} \sum_1^N (fluxStor_{top,i} - fluxStor_{all\ level,i})^2} \quad (4)$$

$$normalized\ RMSE = \frac{RMSE}{\sqrt{\frac{1}{N} \sum_1^N (fluxStor_{all\ level,i} - \overline{fluxStor_{all\ level,i}})^2}} \quad (5)$$

where N being the number of data couples $fluxStor_{top,i}$ and $fluxStor_{all\ level,i}$, $fluxStor_{all\ level,i}$ being the i th reference EC storage term and $fluxStor_{top,i}$ being the i th reference EC storage term computed with only top measurement. The overbar represents a time average:

$$\overline{fluxStor_{all\ level,i}} = \frac{1}{N} \sum_1^N fluxStor_{all\ level,i} \quad (6)$$

The fitted slope indicates how close the mean of the EC storage term using only the top-level is compared to the reference EC storage term using all level observations. The R^2 indicates how scattering the estimates are compared to the fitted line, that is the precision. The normalized RMSE is an indicator of both accuracy and precision.

We found that with low fitted slope and large normalized RMSE, using only top level CO₂ measurements underestimate the air storage terms in all three sites (Fig. 3). The fitted slopes were close to 1 for H and LE storage terms at three sites, but still with a bias of -21–1%. The normalized RMSEs for storage H, LE and CO₂ were 35%–62%, 63%–85%, and 83%–92%, respectively. That the normalized RMSEs are

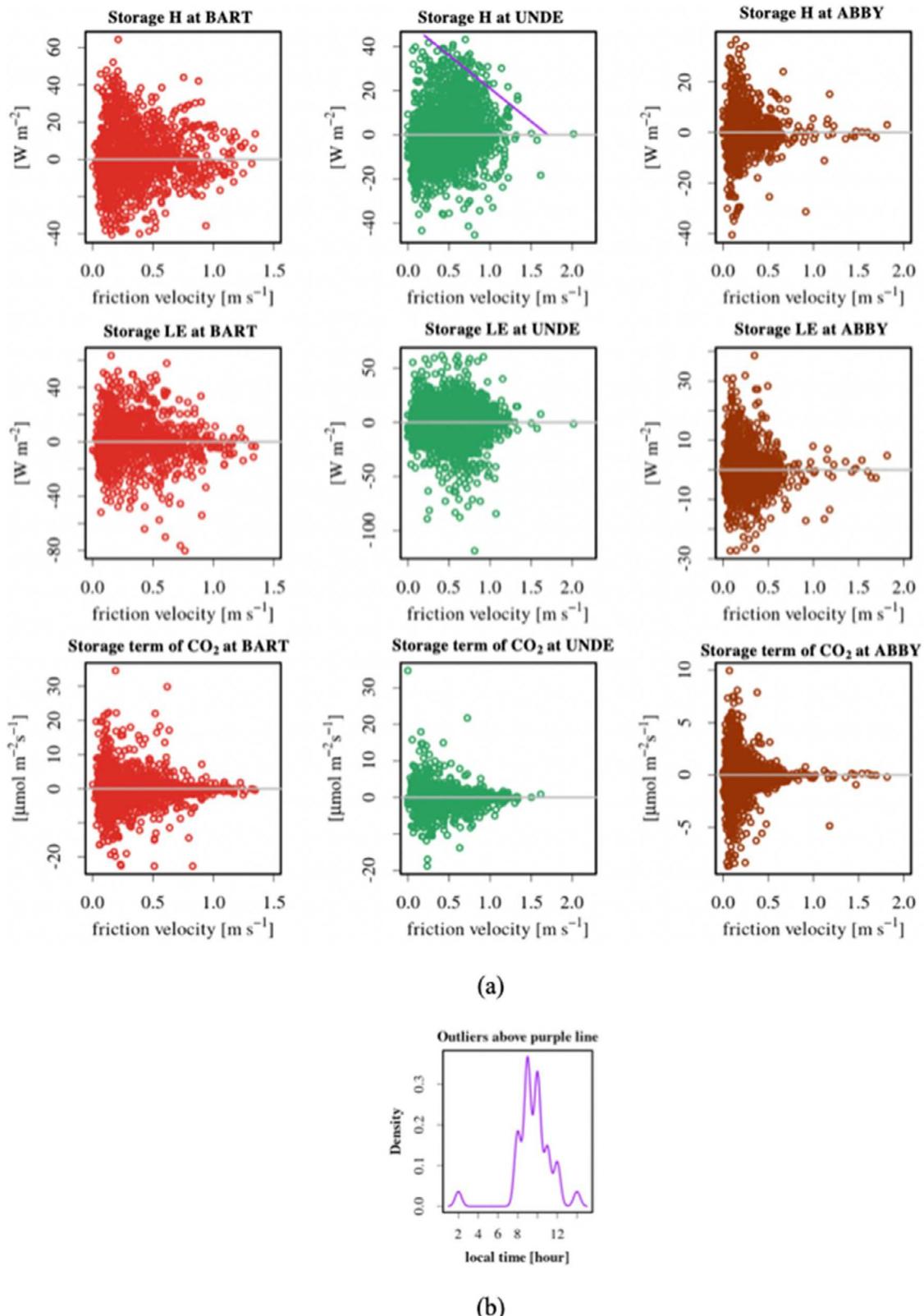


Fig. 6. (a) Scatter plots of H, LE, and CO_2 EC storage term over friction velocity for BART, UNDE and ABBY sites (columns). Gray line is where zero is. (b) the probability density function of outliers above the purple line in EC storage term of H at UNDE. Purple line is defined in Section 3.3.1.

close to 100% indicates that EC storage terms estimated using only top level were not precise. Storage H and LE estimated from only top level exhibit difference across sites, with values closer to the reference EC storage term at UNDE than ABBY and BART.

We then computed the normalized RMSE and fitted slope for the estimated storage term using top level measurements along with randomly chosen one to all levels below the top level (Fig. 4). For all three storage terms, fitted slopes reach 0.98–1.05 when the top level

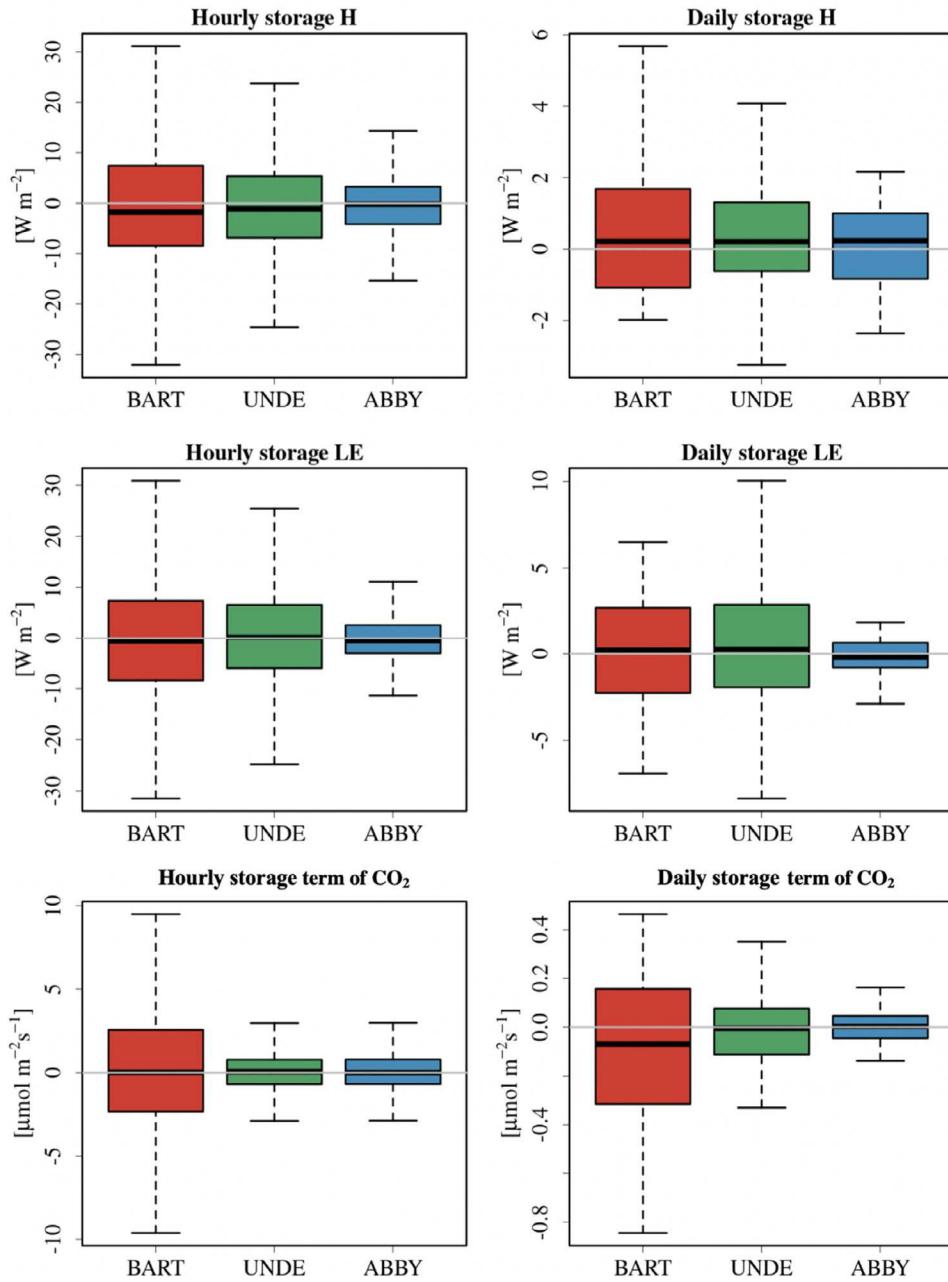


Fig. 7. Box plots for EC storage term of sensible heat (H), latent heat (LE), and CO_2 flux at three sites (BART, UNDE and ABBY) at hourly and daily scales.

measurements as well as another two randomly chosen levels are used. For storage CO_2 term, it is interesting to note that storage term tends to be underestimated when only top measurements used, which is opposite to the 13–18% overestimation from using top measurements and another one randomly chosen level. Fig. 4b shows that normalized RMSE gradually decreases when one level is added each time. At the three sites, the normalized RMSE is still around 20% even with one level missing, that is, Top + 4 levels for BART and UNDE, and Top + 3 levels for ABBY. This indicates that in order to measure storage term accurately and precisely, all levels for the three sites are still necessary. Normalized RMSE is larger at BART than those at ABBY and UNDE sites, suggesting that a larger intensity of vertical profile measurements is more important over a more homogeneous surface.

3.3. Test EC air storage term pattern and significance to net surface-atmosphere exchange

We used the NEON storage term data products, which is released along with this paper, to explore the pattern and importance of EC air storage term to net surface-atmosphere exchange (NSAE) across all three sites. Mean diurnal cycle and monthly averaged EC storage term (stor), turbulent flux (turb), and NSAE for H, LE, and CO_2 flux are calculated across three sites (Fig. 5). To avoid the effect of the different data coverage between day and night, monthly averaged fluxes were aggregated from the mean diurnal cycle. We also explored over what time averaging scale results in zero air storage term, by carrying out a spectral analysis using fast Fourier transformation.

3.3.1. When, where, and to what extent does air storage term matter to net surface-atmosphere exchange?

At these three sites (BART, UNDE, ABBY), air storage term had more

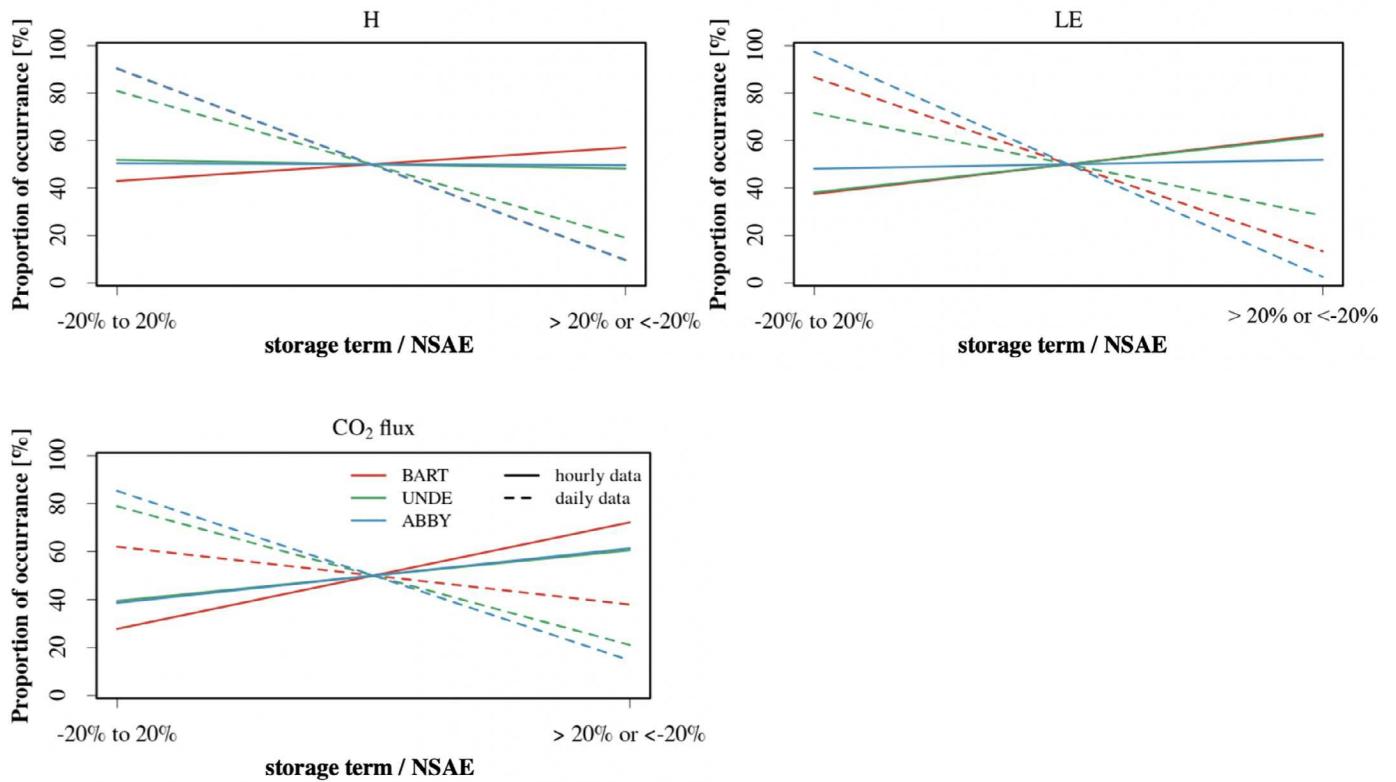


Fig. 8. Data distribution of EC storage term/NSAE for two situations: 1) EC storage term contributed less than 20% magnitude to NSAE; and 2) EC storage term contributed more than 20% magnitude to NSAE at hourly (solid lines) and daily (dash lines) timescales for three sites.

importance for NSAE of H and CO₂ fluxes than for LE (Fig. 5). For all three variables at each site, air storage term peaked in the morning around 8 am local time (positive peak for H and LE, and negative peak for CO₂ flux), which is at the beginning of the development of the convective boundary layer (CBL). As convective boundary layer develops, the temperature gradient brings hot air near surface as well as the tracers within the air to the volume between the surface and top measurements, results in large magnitude of air storage terms. After this peak, the slope of air storage term and turbulent flux were opposite. For example, for H, air storage term trended back toward 0 W m⁻² after 9 am, at the same time, the magnitude of turbulent flux became even larger. We hypothesize that this peak occurred because there was a time delay between the onset of radiative heating and the development of convective boundary layer (CBL) caused by the large temperature gradients. The column between the ground surface and the tower top is more sensitive to the flux changing, especially with the canopy top as a virtual lid, making the EC storage term respond to the surface flux more quickly than turbulent flux.

In all, the storage term in air was relevant at three forest sites, especially below the canopy height. The canopy top can act as a virtual "lid" trapping the surface flux in the form of the storage term in air for a while, and preventing the surface flux from being registered as turbulent flux within the averaging time. This process is likely why the storage term in air peaked between 8 and 9 am and around 4 pm, as the time between onset of radiative heating/cooling and the full development of stronger CBL/initiation of stable boundary layer, and when the turbulent flux and the storage term in air partially exchange into each other. EC storage term is also related to friction velocity, u^* (Fig. 6). EC storage term was usually large when u^* was small, typically during stable conditions when turbulence was insufficient to connect above- and below-canopy air spaces (Aubinet et al., 2000; Janssens et al., 2001; Suyker et al., 2005; Zhao et al., 2006). But there were outliers, e.g. above the purple line ($y > 48-30 \times$) in the subplot of storage H at UNDE, when high EC storage term associated with high u^* measured at

tower top above the canopy. The probability density function of these outliers in Fig. 6b shows that large EC storage term occurred over 8:00–12:00, from the beginning to the full development of the CBL. This is likely because of the decoupling of air flow above and within plant canopies. Furthermore, this indicates potential limitations of univariate data filtering approaches such as u^* thresholding.

Fig. 7 shows box plots for EC storage term of hourly and daily sensible heat (H), latent heat (LE), and CO₂ flux at three sites (BART, UNDE and ABBY). The magnitude of hourly storage H was as large as $\pm 30 \text{ W m}^{-2}$ for H and LE, and $\pm 10 \text{ } \mu\text{mol m}^{-2} \text{ s}^{-1}$ for CO₂ flux. The range of daily EC storage term had a smaller magnitude, but still comparable to monthly NSAE. Although the monthly mean of EC storage term was near zero, hourly and daily EC storage terms had large variation at all three forest sites. The magnitude of EC storage term was usually larger at BART than other two sites probably for two reasons. 1) The EC storage term comprised a larger part of NSAE at the homogeneous sites at hourly temporal scale, as discussed in the above paragraph. 2) The magnitudes of CO₂, LE, and H air storage terms were larger at this mature deciduous forest site compared to the mixed forest site UNDE and the shorter tower young conifer forest site, ABBY.

To understand the relative importance of air storage term, we bin all observations across sites for two conditions according to the contribution of air storage term to NSAE: 1) air storage term contributed more than 20% magnitude to NSAE; and 2) air storage term contributed less than 20% magnitude to NSAE at hourly and daily time scales for the three sites (Fig. 8). Twenty percent was chosen as it is about the amount of energy budget non-closure. Very small NSAE values with small air storage term, e.g. 1 W m⁻² air storage term can be 1000% of 0.1 W m⁻² NSAE. The ratio in this case can create the impression of large air storage term contributions that however are disproportional to their net contribution e.g. to a daily aggregate. However, very small NSAE with large air storage term, e.g. 5 W m⁻² air storage term with 0.1 W m⁻² NSAE indicates that air storage term and turbulent flux exchange to each other, this is when air storage term is very important. In order to

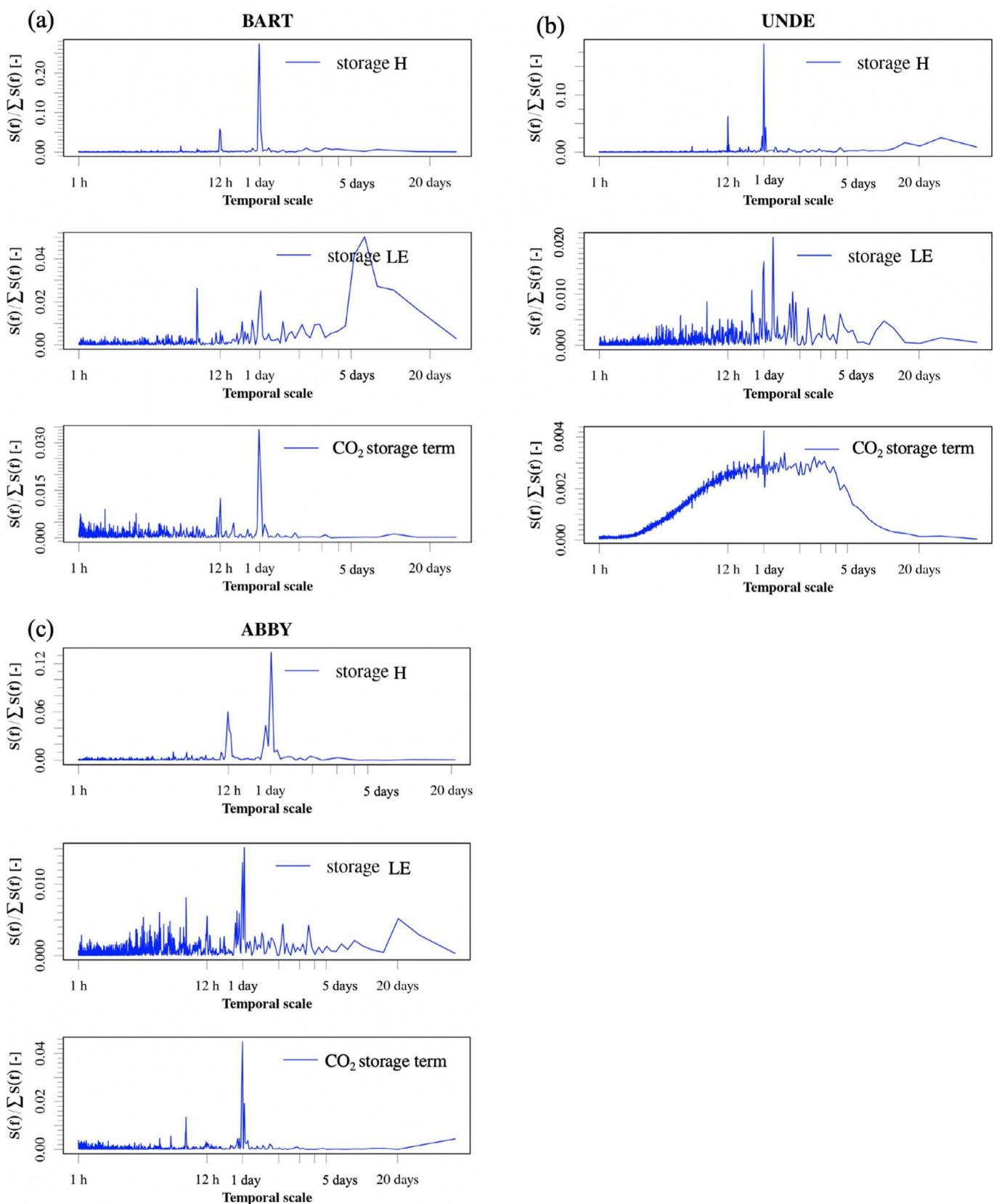


Fig. 9. Spectral plots of EC storage term of sensible heat (H), latent heat (LE), and CO₂ flux for a) BART, b) UNDE, and c) ABBY sites.

consider these two situations, occurrences for which both NSAE and storage magnitude was below 2 W m^{-2} for H and LE, and $0.06 \mu\text{mol m}^{-2} \text{ s}^{-1}$ for CO_2 flux were filtered out. The larger the slope of the line is, the more occurrences in which air storage term contributes $>20\%$ magnitude to NSAE. At the hourly timescale, in 49%–73% of all occurrences air storage term contributed $>20\%$ to NSAE, compared to 10%–37% at the daily timescale. This indicates that air storage term was typically important at all three forest sites at hourly to daily scales, and in particular at the hourly timescale.

3.3.2. When does air storage term average to zero?

Fig. 9 shows that spectral plots of air storage term of sensible heat (H), latent heat (LE), and CO_2 flux for a) BART, b) UNDE, and c) ABBY sites. The spectral energy of EC storage terms consistently peaked at one day temporal scale, indicating that the pattern of EC storage terms throughout the day should not be neglected. For storage H, the energy is 0 at two days frequency, meaning that there is no energy or variance for time average of storage H over 2 days. That is, EC storage term of H average to zero over the course of two days at three sites. Latent heat EC storage terms at all three sites peaked again at the synoptic scale, associated with rainfall events. BART and UNDE had rainfall events with at least 1 mm/hour in consecutive 2–7 days, while ABBY had rainfall events with one hour at least 1 mm/hour in consecutive 24 days (data source: <https://www.neonscience.org/field-sites>). At the heterogeneous UNDE site the energy of storage CO_2 flux spanned from three hours to several days. This is possibly the result of foregoing the homogeneity assumption (Section 1) and corresponding flux modulation resulting from spatial variations in the surface CO_2 flux field in combination with terrain effects. In all, EC storage term of H average to zero over the course of two days at three sites, EC storage term of CO_2 average to zero over two days at BART and ABBY, but over one week at UNDE. EC storage term of LE average to zero over the course of one week at BART and UNDE, and over >20 days at ABBY due to the effect of rainfall events.

4. Summary and conclusions

In this paper, we derive and publish the NEON standardized air storage term measurement setup, eddy-covariance (EC) storage exchange software eddy4R.stor, and EC storage term data product format. The software eddy4.stor package is developed and released through the NEON DevOps model, which ensures portable, reproducible and extensible software. ECSE storage data products, which consistently measured and calculated across 47 NEON sites, are ready at the NEON Data Portal in a near-real-time pipeline, i.e. data product available within 30 days from data acquisition.

The usefulness and capability of these resources were demonstrated with three field sites example, BART, ABBY, and UNDE. We first used the three field sites to test how many levels are necessary for ascertaining air storage term. We found that using only top level measurements resulted in a bias of -21% – 1% for storage H and LE at the three sites. For CO_2 storage term, using only the top measurements underestimated the storage term by 36%–55%, which is opposite with the 13%–18% overestimation when two levels were used. Further, missing a single level can result in a 20% normalized RMSE for all three storage terms at three sites, reflecting that all levels are necessary to measure storage terms accurately and precisely. Intensity of vertical profile measurements is found to be more important over the more homogeneous field site. The second test shows that the storage term had strong diurnal cycles: peaking at early mornings (8:00–10:00), afternoons around 16:00, and during intermittent turbulence periods. At forest sites, we noticed evidence that turbulent fluxes were decoupled with the canopy top, which acts as a lid above the surface where the majority of ecological functioning occurs. These findings suggest that air storage term cannot be neglected at diurnal or daily timescale or over tall canopies.

Future work will focus on a comprehensive comparison of the algorithm implementation in this study with previously published EC storage term algorithms, such as eddyPro (LI-COR, Inc. Lincoln, USA) and Integrated Carbon Observation System (ICOS, [Montagnani et al., 2018](#)). Future work is needed to explore the possibility of relaxing the steady-state assumption inherent to EC, which can promise more reliable, observation-based insight on the diurnal patterns of energy, water, and carbon fluxes. This can be further progressed by exploring the impact of different possible algorithmic choices across software on EC storage term, including the special case of u^* filtering. Such progress would profit our understanding of carbon flux partitioning, ecosystem function and modeling, and energy balance.

We derive and release one of the first community resources to consistently investigate the EC storage term in air and thus improve the overall reliability of flux measurements. After consistent and standardized measuring and processing across NEON 47 sites, EC storage term data products as well as the algorithm package, eddy4R, are derived and released to the public through the NEON Data Portal and Github open-source repository. Resources and results presented in this study highlight the significance of storage term for the community and should promote consistent usage of EC storage term as a key component of high-level EC data products in the climate and carbon cycle research.

Acknowledgments

The National Ecological Observatory Network is a project sponsored by the National Science Foundation and managed under cooperative agreement by Battelle. This material is based upon work supported by the National Science Foundation [grant DBI-0752017]. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author and do not necessarily reflect the views of the National Science Foundation. ARD and KX acknowledge support from Battelle Contract No. 3010-0401-000 made to the University of Wisconsin-Madison.

Code and data availability

The eddy4R.stor R-package that operationally produces the EC storage term data products for NEON is publicly released here (<https://w3id.org/kxu/eddy4R.stor>). The example application described in Section 3 are written in the Github private repository, <https://w3id.org/kxu/manuscriptCode>, which is available upon request.

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at [doi:10.1016/j.agrformet.2019.107734](https://doi.org/10.1016/j.agrformet.2019.107734).

References

- Andrews, A., Kofler, J., Trudeau, M., Williams, J., Neff, D., Masarie, K., ... Zhao, .C., 2014. CO_2 , CO , and CH_4 measurements from tall towers in the NOAA earth system research laboratory's global greenhouse gas reference network: instrumentation, uncertainty analysis, and recommendations for future high-accuracy greenhouse gas monitoring efforts. *Atmos. Meas. Tech.* 7 (2), 647–687.
- Aubinet, M., Berbigier, P., Bernhofer, C., Cescatti, A., Feigenwinter, C., Granier, A., ... Sedlak, P., 2005. Comparing CO_2 storage and advection conditions at night at different carboeuroflux sites. *Bound. Layer Meteorol.* 116 (1), 63–93. <https://doi.org/10.1007/s10546-004-7091-8>. Retrieved from. <https://doi.org/10.1007/s10546-004-7091-8>.
- Aubinet, M., 2008. EDDY covariance CO_2 flux measurements in nocturnal Conditions: an analysis of the problem. *Ecol. Appl.* 18 (6), 1368–1378. <https://doi.org/10.1890/06-1336.1>.
- Aubinet, M., Vesala, T., Papale, D., 2012. *Eddy Covariance: A Practical Guide to Measurement and Data Analysis*. Springer.
- Baldocchi, D., 2008. 'Breathing' of the terrestrial biosphere: lessons learned from a global network of carbon dioxide flux measurement systems. *Aust. J. Bot.* 56 (1), 1–26.
- Brock, F.V., 1986. A nonlinear filter to remove impulse noise from meteorological data. *J. Atmos. Ocean. Technol.* 3 (1), 51–58. [https://doi.org/10.1175/1520-0426\(1986\)003<0051:ANFTRI>2.0.CO;2](https://doi.org/10.1175/1520-0426(1986)003<0051:ANFTRI>2.0.CO;2).

Burns, S.P., Blanken, P.D., Turnipseed, A.A., Hu, J., Monson, R.K., 2015. The influence of warm-season precipitation on the diel cycle of the surface energy balance and carbon dioxide at a Colorado subalpine forest site. *Biogeosciences* 12, 7349–7377. <https://doi.org/10.5194/bg-12-7349-2015>.

Desai, A.R., 2014. Influence and predictive capacity of climate anomalies on daily to decadal extremes in canopy photosynthesis. *Photosyn. Res.* 119 (1–2), 31–47. <https://doi.org/10.1007/s11120-013-9925-z>.

Eshonkulov, R., Poyda, A., Ingwersen, J., Pulatov, A., Streck, T., 2019. Improving the energy balance closure over a winter wheat field by accounting for minor storage terms. *Agric. For. Meteorol.* 264, 283–296. <https://doi.org/10.1016/j.agrformet.2018.10.012>.

Falge, E., Baldocchi, D., Olson, R., Anthoni, P., Aubinet, M., Bernhofer, C., ... Dolman, H., 2001. Gap filling strategies for defensible annual sums of net ecosystem exchange. *Agric. For. Meteorol.* 107 (1), 43–69.

Finnigan, J., 2006. The storage term in eddy flux calculations. *Agric. For. Meteorol.* 136 (3), 108–113. <https://doi.org/10.1016/j.agrformet.2004.12.010>.

Foken, T., 2008. "The energy balance closure problem: an overview. *Ecol. Appl.* 18 (6), 1351–1367.

Foken, T., Wichura, B., 1996. Tools for quality assessment of surface-based flux measurements. *Agric. For. Meteorol.* 78 (1), 83–105. [https://doi.org/10.1016/0168-1923\(95\)02248-1](https://doi.org/10.1016/0168-1923(95)02248-1).

Janssens, I., Lankreijer, H., Matteucci, G., Kowalski, A., Buchmann, N., Epron, D., ... Grünwald, T., 2001. Productivity overshadows temperature in determining soil and ecosystem respiration across European forests. *Glob. Chang. Biol.* 7 (3), 269–278.

Juang, J.Y., Katul, G.G., Siqueira, M., Stoy, P.C., Palmroth, S., McCarthy, H.R., ... Oren, R., 2006. Modeling nighttime ecosystem respiration from measured CO₂ concentration and air temperature profiles using inverse methods. *J. Geophys. Res.* 111 (D8).

Leuning, R., van Gorsel, E., Massman, W.J., Isaac, P.R., 2012. Reflections on the surface energy imbalance problem. *Agric. For. Meteorol.* 156, 65–74. <https://doi.org/10.1016/j.agrformet.2011.12.002>.

Lindroth, A., Molder, M., Lagergren, F., 2010. Heat storage in forest biomass improves energy balance closure. *Biogeosciences* 7, 301–313. <https://doi.org/10.5194/bg-7-301-2010>.

Mahecha, M.D., Gans, F., Sippel, S., Donges, J.F., Kaminski, T., Metzger, S., ... Zscheischler, J., 2017. Detecting impacts of extreme events with ecological in situ monitoring networks. *Biogeosciences* 14 (18), 4255–4277. <https://doi.org/10.5194/bg-14-4255-2017>.

Massman, W.J., Lee, X., 2002. Eddy covariance flux corrections and uncertainties in long-term studies of carbon and energy exchanges. *Agric. For. Meteorol.* 113 (1), 121–144. [https://doi.org/10.1016/S0168-1923\(02\)00105-3](https://doi.org/10.1016/S0168-1923(02)00105-3).

Metzger, S., Ayres, E., Durden, D., Florian, C., Lee, R., Lynch, C., ..., Zulueta, R.C. (2019). From NEON field sites to data portal: a community resource for surface-atmosphere research comes online.

Metzger, S., 2018. Surface-atmosphere exchange in a box: making the control volume a suitable representation for in-situ observations. *Agric. For. Meteorol.* (Massman special issue).

Metzger, S., Durden, D., Sturtevant, C., Luo, H., Pingintha-Durden, N., Sachs, T., ... Desai, A.R., 2017. eddy4R 0.2.0: a DevOps model for community-extensible processing and analysis of eddy-covariance data based on R, Git, Docker, and HDF5. *Geosci. Model Dev.* 10 (9), 3189–3206. <https://doi.org/10.5194/gmd-10-3189-2017>.

Monson, R.K., Sparks, J.P., Rosenstiel, T.N., Scott-Denton, L.E., Huxman, T.E., Harley, P.C., ... Hu, J., 2005. Climatic influences on net ecosystem CO₂ exchange during the transition from wintertime carbon source to springtime carbon sink in a high-elevation, subalpine forest. *Oecologia* 146 (1), 130–147. <https://doi.org/10.1007/s00442-005-0169-2>.

Montagnani, L., Grünwald, T., Kowalski, A., Mammarella, I., Merbold, L., Metzger, S., ..., Siebicke12, L. (2018). Estimating the storage term in eddy covariance measurements: the ICOS methodology.

Nicolini, G., et al., 2018. Impact of CO₂ storage flux sampling uncertainty on net ecosystem exchange measured by eddy covariance. *Agric. For. Meteorol.* 248, 228239. <https://doi.org/10.1016/j.agrformet.2017.09.025>.

Novick, K.A., Biederman, J.A., Desai, A.R., Litvak, M.E., Moore, D.J.P., Scott, R.L., Torn, M.S., 2018. The Ameriflux network: a coalition of the willing. *Agric. For. Meteorol.* 249 (Supplement C), 444–456. <https://doi.org/10.1016/j.agrformet.2017.10.009>.

Papale, D., Valentini, R., 2003. A new assessment of European forests carbon exchanges by eddy fluxes and artificial neural network spatialization. *Glob. Chang. Biol.* 9 (4), 525–535.

Raupach, M.R., 1988. *Canopy Transport Processes*. Berlin, Heidelberg.

Reed, D.E., Frank, J.M., Ewers, B.E., Desai, A.R., 2018. Time dependency of eddy covariance site energy balance. *Agric. For. Meteorol.* 249, 467–478. <https://doi.org/10.1016/j.agrformet.2017.08.008>.

Schwandner, F.M., Gunson, M.R., Miller, C.E., Carn, S.A., Eldering, A., Krings, T., ... Podolske, J.R., 2017. Spaceborne detection of localized carbon dioxide sources. *Science* 358 (6360). <https://doi.org/10.1126/science.aam5782>.

Starkenburg, D., Metzger, S., Fochesatto, G.J., Alfieri, J.G., Gens, R., Prakash, A., Cristóbal, J., 2016. Assessment of despiking methods for turbulence data in micrometeorology. *J. Atmos. Ocean. Technol.* 33 (9), 2001–2013.

Suyker, A.E., Verma, S.B., Burba, G.G., Arkebauer, T.J., 2005. Gross primary production and ecosystem respiration of irrigated maize and irrigated soybean during a growing season. *Agric. For. Meteorol.* 131 (3–4), 180–190.

Swenson, S.C., Burns, S., Lawrence, D., 2019. The impact of biomass heat storage on the canopy energy balance and atmospheric stability in the community land model. *J. Adv. Model. Earth Syst.* 11, 83–98. <https://doi.org/10.1029/2018MS001476>.

Tang, X., Li, H., Desai, A.R., Nagy, Z., Luo, J., Kolb, T.E., ... Ammann, C., 2014. How is water-use efficiency of terrestrial ecosystems distributed and changing on earth? *Sci. Rep.* 4, 7483. <https://doi.org/10.1038/srep07483>. <http://www.nature.com/articles/srep07483#supplementary-information>.

Taylor, G.I., 1938. The spectrum of turbulence. *Proc. R. Soc. London A Math. Phys. Sci.* 164 (919), 476–490.

van Gorsel, E., Delpierre, N., Leuning, R., Black, A., Munger, J.W., Wofsy, S., ... Wharton, S., 2009. Estimating nocturnal ecosystem respiration from the vertical turbulent flux and change in storage of CO₂. *Agric. For. Meteorol.* 149 (11), 1919–1930. <https://doi.org/10.1016/j.agrformet.2009.06.020>.

van Gorsel, E., Leuning, R., Cleugh, H.A., Keith, H., Suni, T., 2007. Nocturnal carbon efflux: reconciliation of eddy covariance and chamber measurements using an alternative to the u-threshold filtering technique. *Tellus B* 59 (3), 397–403. <https://doi.org/10.1111/j.1600-0889.2007.00252.x>.

WMO, 2014. Report of the 17th WMO/IAEA Meeting on Carbon Dioxide, Other Greenhouse Gases and Related Tracers Measurement Techniques (GGMT-2013). Beijing, China, 10–13 June 2013. World Meteorological Organization, Geneva, Switzerland GAW 213, available at: http://library.wmo.int/pmb Ged/gaw_213_en.pdf.

Wolf, S., Yin, D., Roderick, M.L., 2017. Using radiative signatures to diagnose the cause of warming during the 2013–2014 Californian drought. *J. Hydrol. (Amst)* 553, 408–418. <https://doi.org/10.1016/j.jhydrol.2017.07.015>.

Xu, K., Metzger, S., Desai, A.R., 2017. Surface-atmosphere exchange in a box: space-time resolved storage and net vertical fluxes from tower-based eddy covariance. *Agric. For. Meteorol.* <https://doi.org/10.1016/j.agrformet.2017.10.011>.

Zhao, L., Li, Y., Xu, S., Zhou, H., Gu, S., Yu, G., Zhao, X., 2006. Diurnal, seasonal and annual variation in net ecosystem CO₂ exchange of an alpine shrubland on Qinhai-Tibetan plateau. *Glob. Chang. Biol.* 12 (10), 1940–1953.