Stable isotopes contain substantial additive information about terrestrial carbon and water cycling.

Bonan Li[a,b,c,d] Stephen P. Good[a,b], Richard P. Fiorella[e,f,g], Catherine E. Finkenbiner[a,b], Gabriel J. Bowen[e,f], David C. Noone[h], Christopher J. Still[i], William R.L. Anderegg[f,j,h]

[a]Departement of Biological & Ecological Engineering, Oregon State University
[b]Water Resources Graduate Program, Oregon State University
[c]College of Earth Ocean and Atmospheric Sciences, Oregon State University
[d]Department of Biological & Agricultural Engineering, University of Arkansas
[e]Department of Geology and Geophysics, University of Utah
[f]Global Change and Sustainability Center, University of Utah
[g]Earth and Environmental Sciences Division, Los Alamos National Laboratory
[h]Department of Physics, University of Auckland
[i]Department of Forest Ecosystems and Society, Oregon State University
[j]School of Biological Sciences, University of Utah
[h]Wilkes Center for Climate Science and Policy, University of Utah
Corresponding author: Bonan Li

Abstract

Stable isotope ratios of H (δ^2H), O ($\delta^{18}O$), and C ($\delta^{13}C$) are linked to key biogeochemical process of the water and carbon cycles; however, the degree to which isotope associated processes are reflected in ecosystem flux observations remains unquantified. Here through formal information assessment, new measurements of $\delta^{13}C$ of net ecosystem exchange (*NEE*) as well as δ^2H and $\delta^{18}O$ of latent heat (*LH*) fluxes across the United States National Ecological Observation Network are used to determine conditions under which isotope measurements are informative of environmental exchanges. We find all three isotopic datasets individually contain comparable amounts of information about *NEE* and *LH* fluxes as wind speed observations. Such information from isotope measurements is largely unique. Generally, $\delta^{13}C$ provides more information about *LH* as aridity increases or mean annual precipitation decreases; δ^2H provides more information about *LH* as temperatures or mean annual precipitation decreases, and also provides more information about *NEE* as temperatures decrease. These results demonstrate isotopic variability reflecting biophysical controls on *LH*, and to a lesser extent *NEE*, fluxes is stronger under low precipitation, arid, and cooler conditions. The patterns identified in this study are expected to aid in modeling and data interpretation efforts focused on constraining carbon and water cycles mechanisms.

Keywords: isotope, carbon flux, water flux, NEON, information theory

1. Introduction

Understanding the interactions and drivers of water and carbon exchanges between terrestrial ecosystems and the atmosphere is crucial to illuminate processes driving Earth's current climate as well as forecasting impacts of future change on ecosystems and the climate itself [1,2]. To date, significant efforts have been made to monitor terrestrial carbon and water fluxes, including the widespread development of macroscale eddy covariance (EC) networks to measure ecosystem fluxes [3,4]. EC flux towers can measure continuous net ecosystem exchange (*NEE*) of CO_2 between the land surface and atmosphere at various frequency time domains. Similarly, EC measurements of latent heat flux (*LH*), representing evaporation and transpiration from soils, water bodies, and plant canopies, provides valuable information for understanding regional and global water budgets as well as agricultural applications [5,6]. Flux measurements have been used for a variety of environmental applications such as calibrating and validating remotely sensed flux estimations [7], parameterizing land surface models [8], modeling seasonal crop coefficients [9], and investigating disturbance impacts such as post-fire carbon balance [10]. While measurements of *LH* and *NEE* can quantify fluxes themselves, new kinds of data are needed to refine knowledge of the processes driving these fluxes which are central to the carbon and water cycles.

To improve understanding of Earth system processes, the geoscience community has developed a wide array of advanced measurements to complement EC flux data to help constrain environmental processes. These include studies focused on stable isotope fluxes [11], Carbonyl Sulfide (COS) [12], various radiometric indices such as thermal [13] and solar induced fluorescence (SIF) [14], and even environmental DNA [15]. Prominent among these techniques, naturally occurring water and carbon isotopes measurements have been shown to be a powerful tool for understanding a wide array of ecohydrological and biophysical processes because distinct processes are, and are not, often associated with known isotope transformations (i.e., fractionation effects) [16]. Water isotope ratios (δ^2H and $\delta^{18}O$ in water) have been used to partition evapotranspiration into evaporation and transpiration, as evaporated and transpired fluxes from the same ecosystem may have distinct isotope ratios [17,18]. $\delta^{13}C$ values of CO_2 have also been applied to separate *NEE* into its constituent fluxes, as the isotopic composition of photosynthesis can differ from that of ecosystem respiration [19]. Previous studies of δ^2H, $\delta^{18}O$ and $\delta^{13}C$ examined patterns across distinct ecosystems using cryogenic baths and flask samples, however these approaches are constrained in their ability to provide information about ecosystem-scale processes, which generally requires finer temporal and spatial sampling coverage [20,21]. The development of automated laser spectroscopy systems mounted on EC towers provides new opportunities to obtain long term spatially and temporally resolved atmosphere profiles of these isotopes [22]. The recently launched National Ecological Observatory Network (NEON) provides the first standardized measurements of the stable isotope ratios of H_2O vapor and CO_2 for ecosystems across the USA that can be used to estimate δ^2H and $\delta^{18}O$ of *LH* and $\delta^{13}C$ of *NEE* [23].

The development of advanced ecosystem measurements across networks such as NEON presents new scientific possibilities; yet this also raises the fundamental question of how useful new and often expensive data streams are for constraining targeted environmental processes. Many advanced measurements are made at considerable cost and effort, yet their full value as a source of information beyond traditional meteorological observations (e.g., vapor pressure deficit [*VPD*], air temperature [*T*], global radiation [R_g], and windspeed [*u*]), is rarely demonstrated in a formal sense, especially within continental-scale networks where variability in environmental conditions occurs across a much wider range than individual sites. Here we capitalize on recent advances in information theory to assess the information content of NEON stable isotope data. These advances allow for the formal quantification of linear and nonlinear interactions between variables (termed mutual information) [24], as well as approaches to diagnose how unique the information provided by new data sources is relative to others [25,26]. This study addresses three related questions: (1) Do new observations (here δ^2H, $\delta^{18}O$, and $\delta^{13}C$ values) contain useful information about the bulk *NEE* and *LH* fluxes across North America? (2) Can any of the information provided by new (isotope) measurements be obtained from other meteorological variables? And (3) Under which environmental conditions do these new measurements provide the most additional information? In doing so, this study provides a generalizable approach for evaluating the conditions under which novel geoscience data is helpful for understanding the Earth system. It also formally quantifies the conditions under which environmental processes associated with transformations of stable isotope ratios, as measured systematically within continental scale networks, are a greater contribution to overall environmental exchanges. This approach thereby provides key process level benchmarks for advancing research into Earth's integrated carbon and water cycles.

2 Materials and methods

2.1 Study sites and data preparations

This study was conducted at part of terrestrial sites of National Ecological Observatory Network (NEON), which is a continental scale research platform for understanding the ecological responses to climate change, land use change and species invasion [27]. We used the 30-minute aggregated *NEE*, *LH*, global radiation (R_g), air temperature (T), and the two-dimensional wind speed (u) datasets from the NEON's eddy covariance bundled datasets [28]. The vapor pressure deficit (*VPD*) data were derived based on NEON's relative humidity product [29]. These 30-minte variables were gap-filling and further processed to daily scale. More details can be found in Supplemental information. Daily stable isotope ratios of *NEE* and *LH* were obtained from a recently published datasets [30], which was derived based on the surface isotope composition of carbon dioxide and water vapor across NEON sites.

2.2 Information measures

Mutual information is a measure of how two random variables are probabilistically dependent on each other in the unit of bits [24]. Probabilistically, the mutual information can be expressed as:

$$I(\mathrm{X;Y}) = \sum p(\mathrm{x,y}) \log_2 \left(\frac{p(\mathrm{x, y})}{p(\mathrm{x})p(\mathrm{y})}\right) \tag{1}$$

where $p(x)$, p(y), and p(x,y) are the probability density functions of random variables X, Y, and {X,Y} respectively.

The multivariate mutual information of a single random variable (Z) and a set of random variables {X, Y} characterizes the amount of uncertainty in Z that can be reduced by the knowledge of {X, Y} and can be expressed as:

$$I(\mathrm{X,Y;Z}) = \sum p(\mathrm{x, y, z}) \log_2 \left(\frac{p(\mathrm{x, y, z})}{\mathrm{p(x, y)}p(\mathrm{z})}\right) \tag{2}$$

where p(z), p(x,y), and p(x,y,z) are the probability density functions of variables Z, {X,Y}, and {X,Y,Z}, respectively and were estimated using a kernel density estimation (KDE) method with a gaussian kernel and Silverman bandwidth selection method [31]. We rescaled each data point to a common range of [0, 1] before using KDE. We then evaluate the probability density functions from 0 to 1 with a step size of 0.05.

We computed the pairwise mutual information [e.g., I(*NEE*;*VPD*), I(*LH*;*VPD*) .etc] shared among *VPD*, T, R_g, u, $\delta^{13}C$, $\delta^{2}H$, and d about *NEE* and *LH* iteratively. Due to the limitation of isotope datasets, we computed the mutual information of each variable with the *NEE* and *LH* by subsampling 100 data points without replacement 500 times to ensure constituent data counts in mutual information calculations. Then, the mutual information of the variable of interest and the flux is computed as the average mutual information across 500 resamplings. The mutual information contents computed above are tested for statistical significance (refer to Supplemental information for details).

2.3 Partial information decomposition

The multivariate mutual information can be decomposed into different informational components via a partial information decomposition framework (PID) [25,26,32]. The PID can decompose I(X,Y;Z) into: (1) unique information (U) that is only provided by X or Y solely to the Z; (2) synergistic information (S) that is the information provide to the Z when X and Y act jointly; (3) redundant information (R) that is the overlapping information provided both by X and Y to the Z [33]. The PID framework can be formulated as

$$I(\mathrm{X,Y;\ Z}) = \mathrm{U_X} + \mathrm{U_Y} + \mathrm{R} + \mathrm{S} \tag{3}$$

$$I(\mathrm{X;\ Z}) = \mathrm{U_X} + \mathrm{R} \tag{4}$$

$$I(\mathrm{Y;\ Z}) = \mathrm{U_Y} + \mathrm{R} \tag{5}$$

Where $\mathrm{U_X}$ and $\mathrm{U_Y}$ are the unique information of X and Y to Z, respectively. R and S are the redundant and synergistic information of X and Y to Z, respectively. All PID components are non-negative real numbers in unit of bits[33].

In this study, we quantified the information flow between each flux and each isotope flux ratio by leveraging the PID framework [25]. We defined the decomposed information components that the isotope ratios provided to the bulk fluxes as the averaged unique information across all meteorological variables (*VPD*, *T*, R_g, and *u*). As with computing the individual mutual information, we also subsampled 100 data points from each dataset without replacement 500 times. The partial information components of the isotopes were then computed as the averaged information components from 500 iterations. The significance tests were performed similarly to mutual information (refer to Supplemental information for details).

3. Results

Informational analysis shows that isotope data ($\delta^{13}C$, $\delta^{2}H$, and *d*) and traditional meteorological data (R_g, *T*, *VPD*, *u*) each contain significant information about temporal variation in *NEE* and *LH* fluxes (Fig. 1) throughout the NEON sites. We find that R_g, *T*, and *VPD* observations consistently contain more information about environmental fluxes than either isotope data or wind speed (*u*), which provides comparable amount information about *NEE* and *LH* fluxes (Fig. 1). Though the information provided by R_g is larger than the information from *u* and the isotopes, *u* is nevertheless one of the well-established drivers of surface-atmosphere water and carbon exchange and is commonly measured at meteorological stations worldwide [34].

In general, individual variables tend to share more information with *LH* than *NEE* (Fig. 1). This indicates that *LH* is generally more easily constrained and predicted based on these environmental observations, possibly because it more strongly captures isotopic differences in the contributing one-way flux compared to *NEE* which is the net sum of two opposing fluxes with less distinct isotope ratios. Instead of $\delta^{13}C$ values best constraining *NEE* and $\delta^{2}H$ or *d* values best constraining *LH,* we find that $\delta^{2}H$ values on average provide slightly more mutual information than $\delta^{13}C$ values for both *NEE* and *LH* fluxes*;* however, both these (i.e., $\delta^{2}H$ and $\delta^{13}C$) are more informative than *d.* The amount of information that can be inferred from isotopes (and other variables) about *NEE* and *LH* is highly unlikely to be obtained by random processes ($p < 0.01$).

We decomposed and evaluated the multivariate mutual information between environmental fluxes, isotope ratios, and other variables (Fig. 2). These results demonstrate that most of the information provided by the isotopes about *NEE* and *LH* is unique to these measurements ($\delta^{13}C$ and $\delta^{2}H$). This unique information provided by $\delta^{13}C$ and $\delta^{2}H$ values about *LH* is generally higher than the unique information provided about *NEE.* The unique information provided by $\delta^{13}C$ and $\delta^{2}H$ values is higher than that contained within *d* values for both *LH* and *NEE* fluxes. The unique information is found to vary spatially across the NEON sites (Supplemental Fig. S1). All the unique information provided by the isotope ratios is statistically significant and highly unlikely to be obtained at random ($p < 0.01$).

In addition to the unique information that $\delta^{13}C$, $\delta^{2}H$, and *d* values contain about *NEE* and *LH* fluxes, a smaller amount of synergistic and redundant information is also presented (Supplemental Fig. S2 and S3). Among all the isotopes, the synergistic component of *d* values is slightly larger for *NEE* and $\delta^{13}C$ is marginally larger for *LH*. In general, redundant information tends to be smaller than the unique and synergistic components. The unique and redundant information linking isotopes with *NEE* and *LH* are statistically significant ($p < 0.01$).

The total additional information, represented by the sum of the synergistic information and the unique information, provided by each flux isotope composition to *LH* and *NEE* varies spatially across NEON sites (Fig. 3) The fraction of information for isotopes about *NEE* that is additive, i.e. (U+S)/(U+S+R), is 0.95 for $\delta^{13}C$, 0.92 for $\delta^{2}H$, and 0.99 for *d*, respectively). For *LH,* $\delta^{2}H$ and $\delta^{13}C$ provided more additive information than *d* (Fig. 3A). The fraction of additive information about *LH* is 0.89 for $\delta^{13}C$, 0.84 for $\delta^{2}H$, and 0.94 for *d*, respectively. The additive information of $\delta^{13}C$ and $\delta^{2}H$ relating to *LH* has larger variability among sites than that relating to *NEE* (Fig. 3a-3b and Fig. 3d-3e), and there is less variability in the additive information of *d* about *NEE* (Fig. 3c and Fig. 3f) than in *LH*. All the additive information of these isotopes relating to *NEE* and *LH* is statistically significant ($p < 0.01$).

4. Discussion

Our analysis provides a rigorous evaluation of the quantitative value of isotope ratios to provide useful information about carbon and water fluxes across continental scale gradients. For these bulk fluxes, we showed that the information individually provided by these isotopes was similar to the amount of information provided by wind speed measurements, while providing less information than atmospheric vapor pressure deficit, air temperature, and radiation measurements. The meteorological observations evaluated here are commonly used to drive forecasts of environmental processes [35,36] and thus serve as a benchmark for environmental data. A prior *NEE* simulation showed that radiation was consistently the most sensitive predictor for the simulation of *NEE* at maze fields with distinct irrigation practices [37]. Similarly, a sensitivity analysis on global evapotranspiration models indicated that net radiation was found to be one of the influential input variables [38]. Our results are consistent with the fundamental notion that solar radiation is the basis for all ecosystem functions [39] (excluding rare energy transformations) and drives most diurnal variation in air temperature and vapor pressure deficit and therefore is more likely to share higher amount of mutual information individually with *LH* and *NEE*, with temperature and moisture levels of secondary importance and isotope metrics and wind speed of tertiary importance.

The meteorological variables evaluated here are known to be inter-related to some extent. For instance, the vapor pressure deficit is strongly dependent on air temperature due to the Clausius-Clapeyron relationship [40] and air temperature is tightly related to the amount of radiation as well as to sensible heat fluxes. Past studies have highlighted how *NEE* and *LH* respond to changes in vapor pressure deficit, air temperature and radiation across various scales, seasons, and ecosystems [41–43]. Vapor pressure deficit was found to have direct effect on surface energy partitioning as high vapor pressure deficit represents high atmosphere demand and hence high *LH* with constant surface conductance [44,45]. Yet, high vapor pressure deficit can reduce stomatal conductance and thereby reduce plant photosynthesis [46]. Wind speed can modulate the rate of evapotranspiration and thereby *LH* [47,48]. The different effect of vapor pressure deficit and wind speed on *LH* may be underrepresented by other metrics but can be captured if evaluated using information theory-based metrics like those explored here.

Information carried by these isotope ratios was found to be unique. It is also crucial to understand how different variables interactively provide information to a target of interest because knowledge of the interactive dependencies between the inputs and outputs of a studied system is fundamental for model uncertainty characterization [49–51]. In fact, one of the challenges for land surface models is increasing process complexity with the integration of a set of sub-models with the expansion of input dimensions [52], which can increase the risk of model "equifinality". Moreover, numerous models have been developed to estimate ecosystem fluxes [53–55]. However, these methods often require some assumptions or simplifications, which can be subject to significant uncertainty [56,57]. In general, it may be more desirable for most of the inputs in a model to provide unique or synergistic pieces of information [58], which can potentially capture different processes relating to the target [32]. Therefore, the construction and simplification of ecosystem models should be towards a direction that maximizes unique information of each input.

The decomposition of the multivariate mutual information between isotopes, other meteorological variables, and the bulk fluxes offers an opportunity to elucidate how much of the information from isotopes is transferred to the bulk fluxes (*NEE* and *LH*). In this study, the portion of unique information from isotopes measurements for carbon and water isotopes was statistically significant suggesting that isotope ratios of the fluxes may influence these fluxes via distinct pathways. We observed inter-site variations in the unique information provided by the isotopes, indicating that the unique information may be dependent on site-specific conditions (e.g., aridity, precipitation). This suggests that the patterns of bulk fluxes can potentially be better characterized and predicted with the isotopes included as an additional constraint.

The additional information provided by isotopes to these bulk fluxes are described by the sum of unique information and synergistic information. Our analysis demonstrate that fusing isotope data products can potentially lead to better monitoring and prediction of *NEE* and *LH* in a process modeling framework, as these isotope datasets provide additional information beyond traditional meteorological variables and are associated with known physical mechanisms. However, the amount of added information of the isotope datasets is likely to vary across sites, climate, and ecosystems. To assess this, we evaluated the additive information of isotopes based on NEON site conditions via a simple linear regression analysis (Fig. 4). We showed that the additive information that $\delta^{13}C$ provides about *LH* is influenced by mean annual precipitation, aridity, and site elevation (Fig. 4d), as indicated by a significant slope value from the linear regression. $\delta^{13}C$ is likely to provide more useful information about *LH* in locations with higher atmospheric evaporative demand relative to precipitation or in locations with less annual precipitation or with higher altitude. The additive information $\delta^{2}H$ provides about *NEE* was shown to be mainly influenced by the site mean annual temperature (Fig. 4b). $\delta^{2}H$ tends to be more informative about *NEE* in locations with cooler climates. Similarly, there is more opportunity for $\delta^{2}H$ to provide additional knowledge about *LH* at locations with cooler climates or less mean annual precipitation (Fig. 4e). No significant relationship was found between the additional information of the *d* provided to either *NEE* or *LH*.

One of key motivations for measuring stable isotopes of water and carbon fluxes is that they may provide a unique constraint across ecosystems, which has not been formally tested until this study, which allow for the partitioning of bulk fluxes into their respective constituents [59–61]. This is because the flux isotope ratios are influenced by distinct biophysical processes, and thus larger amounts of new mutual information between isotopes and environmental fluxes quantifies the conditions under which these processes are more dominate components of overall bulk fluxes. In this light, the trends described above (and in Fig 4) are consistent with prior knowledge of isotope geophysics. For instance, equilibrium fractionation factors are sensitive to temperature, particularly at low values [16], with broad decreases in vapor $\delta^{2}H$ observed poleward at continental scales [62]. Similarly, evaporation is expected to play a larger role in *LH* fluxes under low vegetation, more arid climates [63] , and this study provides a new way to quantify the relative importance of these isotope processes on bulk fluxes.

This analysis is based on current available data products and quality control methods. It may be also worthwhile for future studies to investigate if and how the results vary with more available datasets and a wider range of environmental conditions. However, given the power of isotopes for tackling fundamental problems in carbon and water cycling and projecting the future of terrestrial ecosystem function under a rapidly changing climate [16,64], our results can be useful to provide guidance for improving model results after the incorporation of isotope flux ratios.

Acknowledgements

The authors want to acknowledge the funding support of the United States National Science Foundation (DEB1802885 and DEB1802880).

Author contribution

BL and SPG designed the study. RPF provided flux datasets and gap-filled meteorological datasets and wrote part of the data processing steps in Supplementary material. BL analyzed the data and wrote the manuscript. SPG, RPF, CEF, GJB, DCN, CJS, and WRLA reviewed the manuscript.

Data availability statement

The datasets that are associated with this study is publicly available at https://data.neonscience.org/ and https://www.hydroshare.org/resource/e74edc35d45441579d51286ea01b519f/.

Competing interest statement

The authors declare no conflicts of interest.

References

1. Jung M, Reichstein M, Margolis HA, Cescatti A, Richardson AD, Arain MA, et al. Global patterns of land-atmosphere fluxes of carbon dioxide, latent heat, and sensible heat derived from eddy covariance, satellite, and meteorological observations. J Geophys Res [Internet]. 2011 Sep 3;116:G00J07. Available from: http://doi.wiley.com/10.1029/2010JG001566

2. Piao S, Wang X, Wang K, Li X, Bastos A, Canadell JG, et al. Interannual variation of terrestrial carbon cycle: Issues and perspectives. Glob Chang Biol [Internet]. 2020 Jan 29;26(1):300–18. Available from: https://onlinelibrary.wiley.com/doi/10.1111/gcb.14884

3. Baldocchi D. Measuring fluxes of trace gases and energy between ecosystems and the atmosphere - the state and future of the eddy covariance method. Glob Chang Biol [Internet]. 2014 Dec;20(12):3600–9. Available from: https://onlinelibrary.wiley.com/doi/10.1111/gcb.12649

4. Schimel D, Schneider FD. Flux towers in the sky: global ecology from space. New Phytologist [Internet]. 2019 Oct 3;224(2):570–84. Available from: https://onlinelibrary.wiley.com/doi/10.1111/nph.15934

5. Zhou S, Yu B, Zhang Y, Huang Y, Wang G. Water use efficiency and evapotranspiration partitioning for three typical ecosystems in the Heihe River Basin, northwestern China. Agric For Meteorol [Internet]. 2018 May;253–254:261–73. Available from: https://linkinghub.elsevier.com/retrieve/pii/S016819231830039X

6. Zeng S, Xia J, Chen X, Zou L, Du H, She D. Integrated land-surface hydrological and biogeochemical processes in simulating water, energy and carbon fluxes over two different ecosystems. J Hydrol (Amst) [Internet]. 2020 Mar;582:124390. Available from: https://linkinghub.elsevier.com/retrieve/pii/S0022169419311254

7. Jia Z, Liu S, Xu Z, Chen Y, Zhu M. Validation of remotely sensed evapotranspiration over the Hai River Basin, China. Journal of Geophysical Research: Atmospheres [Internet]. 2012 Jul 16;117(D13):n/a-n/a. Available from: http://doi.wiley.com/10.1029/2011JD017037

8. Williams M, Richardson AD, Reichstein M, Stoy PC, Peylin P, Verbeeck H, et al. Improving land surface models with FLUXNET data. Biogeosciences [Internet]. 2009 Jul 30;6(7):1341–59. Available from: https://bg.copernicus.org/articles/6/1341/2009/

9. Li S, Kang S, Li F, Zhang L. Evapotranspiration and crop coefficient of spring maize with plastic mulch using eddy covariance in northwest China. Agric Water Manag [Internet]. 2008 Nov;95(11):1214–22. Available from: https://linkinghub.elsevier.com/retrieve/pii/S0378377408001169

10. Lupascu M, Akhtar H, Smith TEL, Sukri RS. Post-fire carbon dynamics in the tropical peat swamp forests of Brunei reveal long-term elevated CH 4 flux. Glob Chang Biol [Internet]. 2020 Sep 15;26(9):5125–45. Available from: https://onlinelibrary.wiley.com/doi/10.1111/gcb.15195

11. Dubbert M, Werner C. Water fluxes mediated by vegetation: emerging isotopic insights at the soil and atmosphere interfaces. New Phytologist [Internet]. 2019 Mar 19;221(4):1754–63. Available from: https://onlinelibrary.wiley.com/doi/10.1111/nph.15547

12. Whelan ME, Lennartz ST, Gimeno TE, Wehr R, Wohlfahrt G, Wang Y, et al. Reviews and syntheses: Carbonyl sulfide as a multi-scale tracer for carbon and water cycles. Biogeosciences [Internet]. 2018 Jun 18;15(12):3625–57. Available from: https://bg.copernicus.org/articles/15/3625/2018/

13. Still CJ, Rastogi B, Page GFM, Griffith DM, Sibley A, Schulze M, et al. Imaging canopy temperature: shedding (thermal) light on ecosystem processes. New Phytologist [Internet]. 2021 Jun 2;230(5):1746–53. Available from: https://onlinelibrary.wiley.com/doi/10.1111/nph.17321

14. Guan K, Berry JA, Zhang Y, Joiner J, Guanter L, Badgley G, et al. Improving the monitoring of crop productivity using spaceborne solar-induced fluorescence. Glob Chang Biol [Internet]. 2016 Feb 10;22(2):716–26. Available from: https://onlinelibrary.wiley.com/doi/10.1111/gcb.13136

15. URycki DR, Bassiouni M, Good SP, Crump BC, Li B. The streamwater microbiome encodes hydrologic data across scales. Science of The Total Environment [Internet]. 2022 Nov;849:157911. Available from: https://linkinghub.elsevier.com/retrieve/pii/S0048969722050100

16. Bowen GJ, Good SP. Incorporating water isoscapes in hydrological and water resource investigations. WIREs Water [Internet]. 2015 Mar 16;2(2):107–19. Available from: https://onlinelibrary.wiley.com/doi/10.1002/wat2.1069

17. Xiao W, Wei Z, Wen X. Evapotranspiration partitioning at the ecosystem scale using the stable isotope method—A review. Agric For Meteorol [Internet]. 2018 Dec;263:346–61. Available from: https://linkinghub.elsevier.com/retrieve/pii/S0168192318303009

18. Berkelhammer M, Hu J, Bailey A, Noone DC, Still CJ, Barnard H, et al. The nocturnal water cycle in an open-canopy forest. Journal of Geophysical Research: Atmospheres [Internet]. 2013 Sep 16;118(17):10,225-10,242. Available from: http://doi.wiley.com/10.1002/jgrd.50701

19. Lee SC, Christen A, Black TA, Jassal RS, Ketler R, Nesic Z. Partitioning of net ecosystem exchange into photosynthesis and respiration using continuous stable isotope measurements in a Pacific Northwest Douglas-fir forest ecosystem. Agric

For Meteorol [Internet]. 2020 Oct;292–293:108109. Available from: https://linkinghub.elsevier.com/retrieve/pii/S0168192320302112

20. Orlowski N, Breuer L, Angeli N, Boeckx P, Brumbt C, Cook CS, et al. Inter-laboratory comparison of cryogenic water extraction systems for stable isotope analysis of soil water. Hydrol Earth Syst Sci. 2018 Jul 6;22(7):3619–37.

21. Gemery PA, Trolier M, White JWC. Oxygen isotope exchange between carbon dioxide and water following atmospheric sampling using glass flasks. Journal of Geophysical Research: Atmospheres. 1996 Jun 20;101(D9):14415–20.

22. Fiorella RP, Good SP, Allen ST, Guo JS, Still CJ, Noone DC, et al. Calibration Strategies for Detecting Macroscale Patterns in NEON Atmospheric Carbon Isotope Observations. J Geophys Res Biogeosci. 2021 Mar 26;126(3).

23. Finkenbiner CE, Li B, Spencer L, Butler Z, Haagsma M, Fiorella RP, et al. The NEON Daily Isotopic Composition of Environmental Exchanges Dataset. Sci Data. 2022 Dec 21;9(1):353.

24. Cover TM, Thomas JA. Elements of Information Theory [Internet]. Wiley; 2005. Available from: https://onlinelibrary.wiley.com/doi/book/10.1002/047174882X

25. Goodwell AE, Kumar P. Temporal information partitioning: Characterizing synergy, uniqueness, and redundancy in interacting environmental variables. Water Resour Res [Internet]. 2017 Jul 24;53(7):5920–42. Available from: https://onlinelibrary.wiley.com/doi/10.1002/2016WR020216

26. Williams PL, Beer RD. Nonnegative Decomposition of Multivariate Information. 2010 Apr 14; Available from: http://arxiv.org/abs/1004.2515

27. Barnett DT, Adler PB, Chemel BR, Duffy PA, Enquist BJ, Grace JB, et al. The plant diversity sampling design for The National Ecological Observatory Network. Ecosphere [Internet]. 2019 Feb 25;10(2). Available from: https://onlinelibrary.wiley.com/doi/10.1002/ecs2.2603

28. National Ecological Observatory Network (NEON). Bundled data products - eddy covariance (DP4.00200.001) [Internet]. National Ecological Observatory Network (NEON); 2022. Available from: https://data.neonscience.org

29. National Ecological Observatory Network (NEON). Relative humidity (DP1.00098.001). National Ecological Observatory Network (NEON); 2022.

30. Finkenbiner CE, Li B, Spencer L, Butler Z, Haagsma M, Fiorella RP, et al. The NEON Daily Isotopic Composition of Environmental Exchanges Dataset. Sci Data [Internet]. 2022 Dec 21;9(1):353. Available from: https://www.nature.com/articles/s41597-022-01412-4

31. Silverman BW. Density Estimation for Statistics and Data Analysis [Internet]. Routledge; 2018. Available from: https://www.taylorfrancis.com/books/9781351456173

32. Goodwell AE, Kumar P, Fellows AW, Flerchinger GN. Dynamic process connectivity explains ecohydrologic responses to rainfall pulses and drought. Proceedings of the National Academy of Sciences [Internet]. 2018 Sep 11;115(37). Available from: https://pnas.org/doi/full/10.1073/pnas.1800236115

33. Goodwell AE, Kumar P. Temporal information partitioning: Characterizing synergy, uniqueness, and redundancy in interacting environmental variables. Water Resour Res. 2017 Jul 24;53(7):5920–42.

34. Yusup Y, Liu H. Effects of persistent wind speeds on turbulent fluxes in the water-atmosphere interface. Theor Appl Climatol [Internet]. 2020 Apr 13;140(1–2):313–25. Available from: http://link.springer.com/10.1007/s00704-019-03084-4

35. Cosgrove BA, Lohmann D, Mitchell KE, Houser PR, Wood EF, Schaake JC, et al. Real-time and retrospective forcing in the North American Land Data Assimilation System (NLDAS) project. Journal of Geophysical Research: Atmospheres [Internet]. 2003 Nov 27;108(D22):2002JD003118. Available from: https://onlinelibrary.wiley.com/doi/abs/10.1029/2002JD003118

36. Rodell M, Houser PR, Jambor U, Gottschalck J, Mitchell K, Meng CJ, et al. The Global Land Data Assimilation System. Bull Am Meteorol Soc [Internet]. 2004 Mar;85(3):381–94. Available from: https://journals.ametsoc.org/doi/10.1175/BAMS-85-3-381

37. Safa B, Arkebauer TJ, Zhu Q, Suyker A, Irmak S. Net Ecosystem Exchange (NEE) simulation in maize using artificial neural networks. IFAC Journal of Systems and Control [Internet]. 2019 Mar;7:100036. Available from: https://linkinghub.elsevier.com/retrieve/pii/S2468601817302584

38. Talsma C, Good S, Miralles D, Fisher J, Martens B, Jimenez C, et al. Sensitivity of Evapotranspiration Components in Remote Sensing-Based Models. Remote Sens (Basel) [Internet]. 2018 Oct 9;10(10):1601. Available from: http://www.mdpi.com/2072-4292/10/10/1601

39. Yetemen O, Istanbulluoglu E, Flores-Cervantes JH, Vivoni ER, Bras RL. Ecohydrologic role of solar radiation on landscape evolution. Water Resour Res [Internet]. 2015 Feb;51(2):1127–57. Available from: http://doi.wiley.com/10.1002/2014WR016169

40. Clausius R. Ueber die bewegende Kraft der Wärme und die Gesetze, welche sich daraus für die Wärmelehre selbst ableiten lassen. Annalen der Physik und Chemie [Internet]. 1850;155(4):500–24. Available from: https://onlinelibrary.wiley.com/doi/10.1002/andp.18501550403

41. Chen J, Wen J, Kang S, Meng X, Tian H, Ma X, et al. Assessments of the factors controlling latent heat flux and the coupling degree between an alpine wetland and the atmosphere on the Qinghai-Tibetan Plateau in summer. Atmos Res [Internet]. 2020 Aug;240:104937. Available from: https://linkinghub.elsevier.com/retrieve/pii/S016980951931573X

42. Niu S, Luo Y, Fei S, Yuan W, Schimel D, Law BE, et al. Thermal optimality of net ecosystem exchange of carbon dioxide and underlying mechanisms. New Phytologist [Internet]. 2012 May 7;194(3):775–83. Available from: https://onlinelibrary.wiley.com/doi/10.1111/j.1469-8137.2012.04095.x

43. Gu L, Meyers T, Pallardy SG, Hanson PJ, Yang B, Heuer M, et al. Direct and indirect effects of atmospheric conditions and soil moisture on surface energy partitioning revealed by a prolonged drought at a temperate forest site. J Geophys Res [Internet]. 2006;111(D16):D16102. Available from: http://doi.wiley.com/10.1029/2006JD007161

44. Tong B, Guo J, Xu H, Wang Y, Li H, Bian L, et al. Effects of soil moisture, net radiation, and atmospheric vapor pressure deficit on surface evaporation fraction at a semi-arid grass site. Science of The Total Environment [Internet]. 2022 Nov;849:157890. Available from: https://linkinghub.elsevier.com/retrieve/pii/S0048969722049890

45. Wang P, Li D, Liao W, Rigden A, Wang W. Contrasting Evaporative Responses of Ecosystems to Heatwaves Traced to the Opposing Roles of Vapor Pressure Deficit and Surface Resistance. Water Resour Res [Internet]. 2019 Jun 4;55(6):4550–63. Available from: https://onlinelibrary.wiley.com/doi/10.1029/2019WR024771

46. Grossiord C, Buckley TN, Cernusak LA, Novick KA, Poulter B, Siegwolf RTW, et al. Plant responses to rising vapor pressure deficit. New Phytologist [Internet]. 2020 Jun 20;226(6):1550–66. Available from: https://onlinelibrary.wiley.com/doi/10.1111/nph.16485

47. Yang Y, Cui Y, Bai K, Luo T, Dai J, Wang W, et al. Short-term forecasting of daily reference evapotranspiration using the reduced-set Penman-Monteith model and public weather forecasts. Agric Water Manag [Internet]. 2019 Jan;211:70–80. Available from: https://linkinghub.elsevier.com/retrieve/pii/S0378377418314732

48. Liu X, Zhang D. Trend analysis of reference evapotranspiration in Northwest China: The roles of changing wind speed and surface air temperature. Hydrol Process [Internet]. 2013 Dec 30;27(26):3941–8. Available from: https://onlinelibrary.wiley.com/doi/10.1002/hyp.9527

49. Ruddell BL, Drewry DT, Nearing GS. Information Theory for Model Diagnostics: Structural Error is Indicated by Trade-Off Between Functional and Predictive

Performance. Water Resour Res [Internet]. 2019 Aug 6;55(8):6534–54. Available from: https://onlinelibrary.wiley.com/doi/10.1029/2018WR023692

50. Li B, Good SP. Information-based uncertainty decomposition in dual-channel microwave remote sensing of soil moisture. Hydrol Earth Syst Sci [Internet]. 2021 Sep 17;25(9):5029–45. Available from: https://hess.copernicus.org/articles/25/5029/2021/

51. Gong W, Gupta H V., Yang D, Sricharan K, Hero AO. Estimating epistemic and aleatory uncertainties during hydrologic modeling: An information theoretic approach. Water Resour Res [Internet]. 2013 Apr;49(4):2253–73. Available from: http://doi.wiley.com/10.1002/wrcr.20161

52. Fisher RA, Koven CD. Perspectives on the Future of Land Surface Models and the Challenges of Representing Complex Terrestrial Systems. J Adv Model Earth Syst [Internet]. 2020 Apr 20;12(4). Available from: https://onlinelibrary.wiley.com/doi/10.1029/2018MS001453

53. Wood DA. Net ecosystem carbon exchange prediction and insightful data mining with an optimized data-matching algorithm. Ecol Indic [Internet]. 2021 May;124:107426. Available from: https://linkinghub.elsevier.com/retrieve/pii/S1470160X21000911

54. Su Z. The Surface Energy Balance System (SEBS) for estimation of turbulent heat fluxes. Hydrol Earth Syst Sci [Internet]. 2002 Feb 28;6(1):85–100. Available from: https://hess.copernicus.org/articles/6/85/2002/

55. Veroustraete F, Patyn J, Myneni RB. Estimating net ecosystem exchange of carbon using the normalized difference vegetation index and an ecosystem model. Remote Sens Environ [Internet]. 1996 Oct;58(1):115–30. Available from: https://linkinghub.elsevier.com/retrieve/pii/0034425795002588

56. Papale D, Reichstein M, Aubinet M, Canfora E, Bernhofer C, Kutsch W, et al. Towards a standardized processing of Net Ecosystem Exchange measured with eddy covariance technique: algorithms and uncertainty estimation. Biogeosciences [Internet]. 2006 Nov 27;3(4):571–83. Available from: https://bg.copernicus.org/articles/3/571/2006/

57. Zhao WL, Qiu GY, Xiong YJ, Paw U KT, Gentine P, Chen BY. Uncertainties Caused by Resistances in Evapotranspiration Estimation Using High-Density Eddy Covariance Measurements. J Hydrometeorol [Internet]. 2020 Jun;21(6):1349–65. Available from: https://journals.ametsoc.org/view/journals/hydr/21/6/JHM-D-19-0191.1.xml

58. Wibral M, Priesemann V, Kay JW, Lizier JT, Phillips WA. Partial information decomposition as a unified approach to the specification of neural goal functions.

Brain Cogn [Internet]. 2017 Mar;112:25–38. Available from: https://linkinghub.elsevier.com/retrieve/pii/S027826261530021X

59. Good SP, Soderberg K, Guan K, King EG, Scanlon TM, Caylor KK. δ 2 H isotopic flux partitioning of evapotranspiration over a grass field following a water pulse and subsequent dry down. Water Resour Res [Internet]. 2014 Feb;50(2):1410–32. Available from: http://doi.wiley.com/10.1002/2013WR014333

60. Conrad R, Klose M, Yuan Q, Lu Y, Chidthaisong A. Stable carbon isotope fractionation, carbon flux partitioning and priming effects in anoxic soils during methanogenic degradation of straw and soil organic matter. Soil Biol Biochem [Internet]. 2012 Jun;49:193–9. Available from: https://linkinghub.elsevier.com/retrieve/pii/S0038071712000958

61. Wang L, Caylor KK, Villegas JC, Barron-Gafford GA, Breshears DD, Huxman TE. Partitioning evapotranspiration across gradients of woody plant cover: Assessment of a stable isotope technique. Geophys Res Lett [Internet]. 2010 May;37(9):n/a-n/a. Available from: http://doi.wiley.com/10.1029/2010GL043228

62. Good SP, Noone D, Kurita N, Benetti M, Bowen GJ. D/H isotope ratios in the global hydrologic cycle. Geophys Res Lett [Internet]. 2015 Jun 28;42(12):5042–50. Available from: http://doi.wiley.com/10.1002/2015GL064117

63. Wang L, Good SP, Caylor KK. Global synthesis of vegetation control on evapotranspiration partitioning. Geophys Res Lett [Internet]. 2014 Oct 16;41(19):6753–7. Available from: http://doi.wiley.com/10.1002/2014GL061439

64. Bowling DR, Pataki DE, Randerson JT. Carbon isotopes in terrestrial ecosystem pools and CO 2 fluxes. New Phytologist [Internet]. 2008 Apr 7;178(1):24–40. Available from: https://onlinelibrary.wiley.com/doi/10.1111/j.1469-8137.2007.02342.x

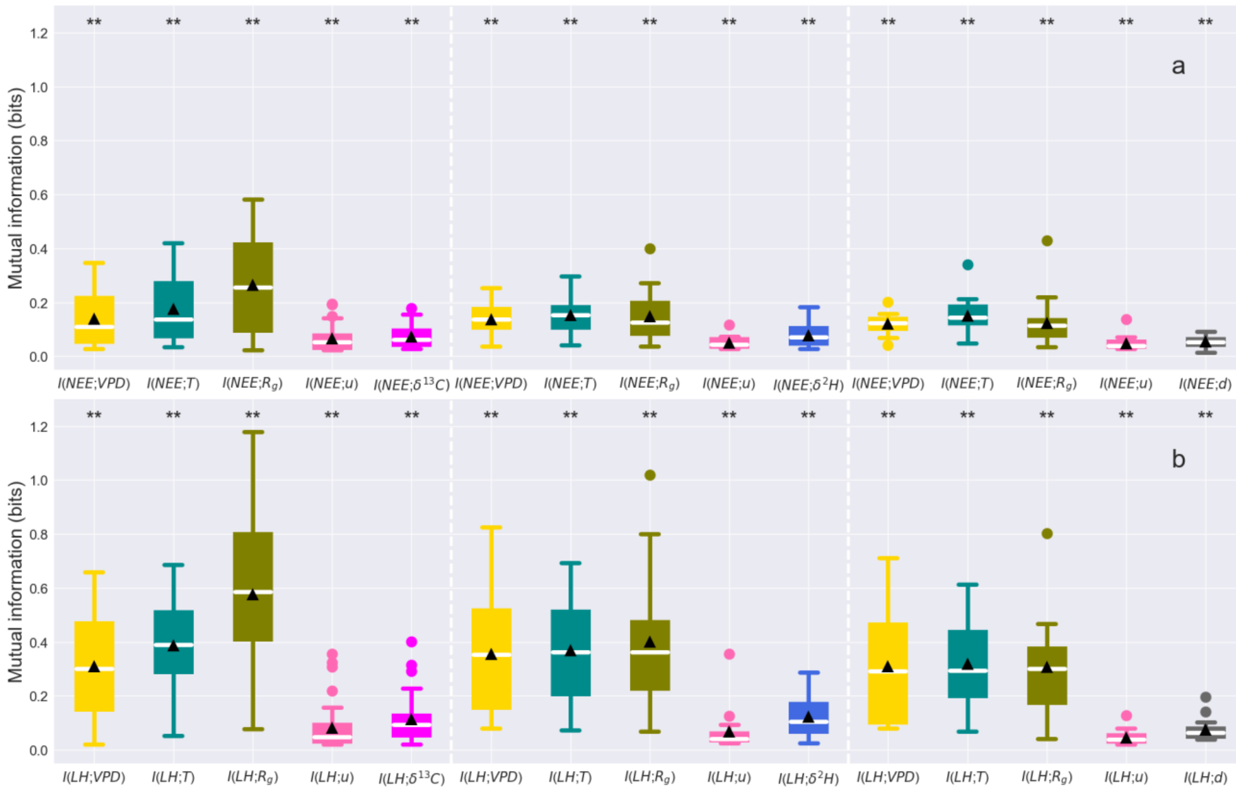

Figure 1 Individual mutual information shared between net ecosystem exchange (*NEE*) and each individual meteorological variable (vapor pressure deficit [*VPD*], air temperature [*T*], global radiation [R_g], windspeed [*u*]) (a). Individual information shared between latent heat flux (*LH*) and each individual meteorological variable (b). The mean and median values of each boxplot are shown as black triangle and white line, respectively. The double asterisk indicates a significant p-value (<0.01).

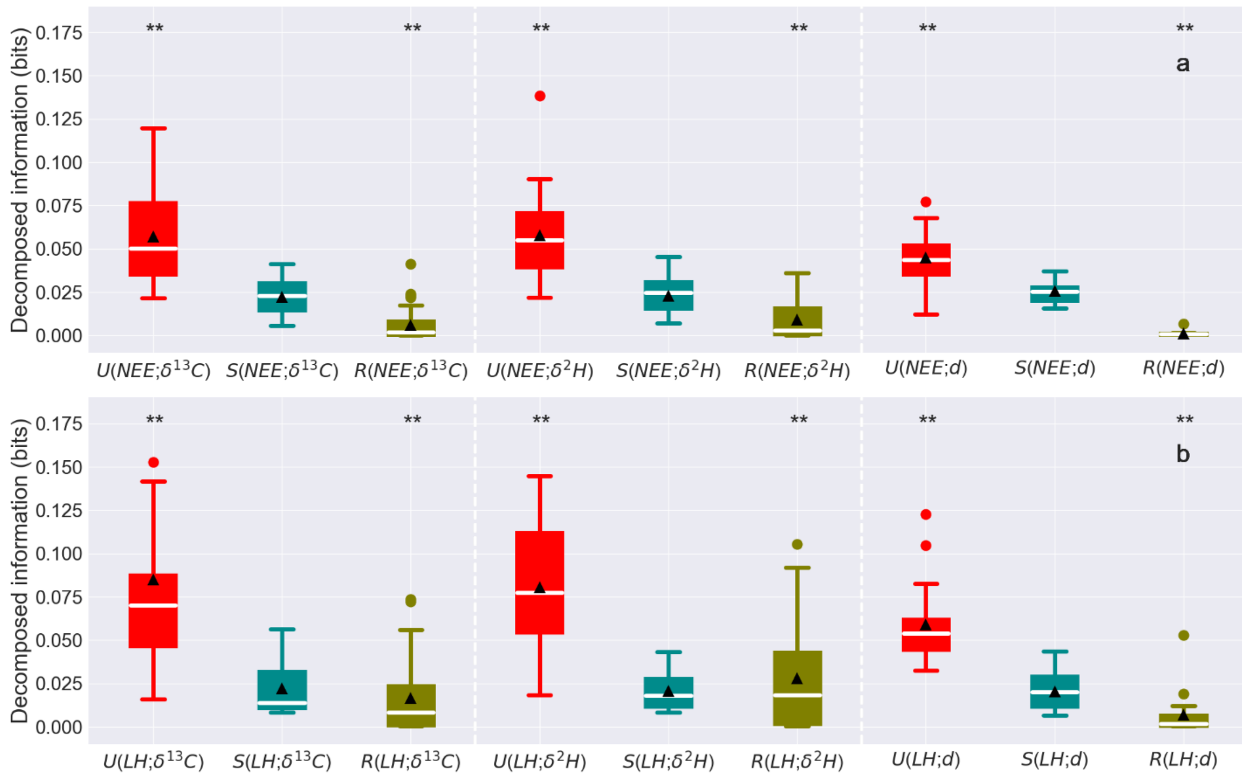

Figure 2 The unique information (*U*), synergistic information (*S*), and redundant information (*R*) of the stable isotope flux ratios on the net ecosystem exchange [*NEE*] (a) and latent heat flux (*LH*) (b) fluxes. The mean and median values of each boxplot are shown as black triangle and white line, respectively. The double asterisk indicates a significant p-value (<0.01).

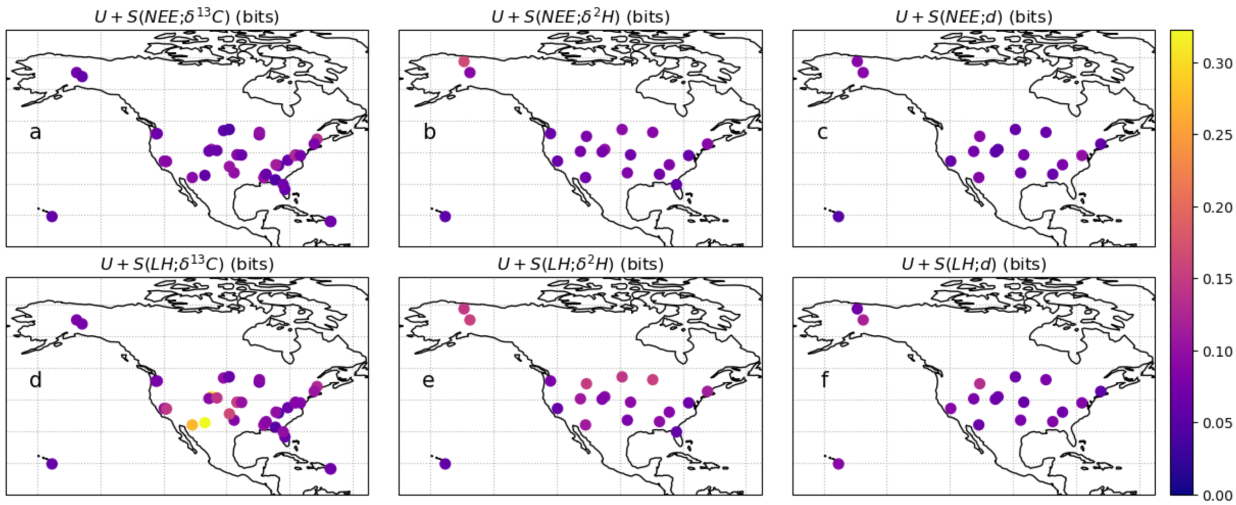

Figure 3 The additive information of $\delta^{13}C$ about net ecosystem exchange (*NEE*) (a) and latent heat flux (*LH*) (d). The additive information of $\delta^{13}H$ about *NEE* (b) and latent heat flux (*LH*) (e). The additive information of *d* about *NEE* (c) and latent heat flux (*LH*) (f).

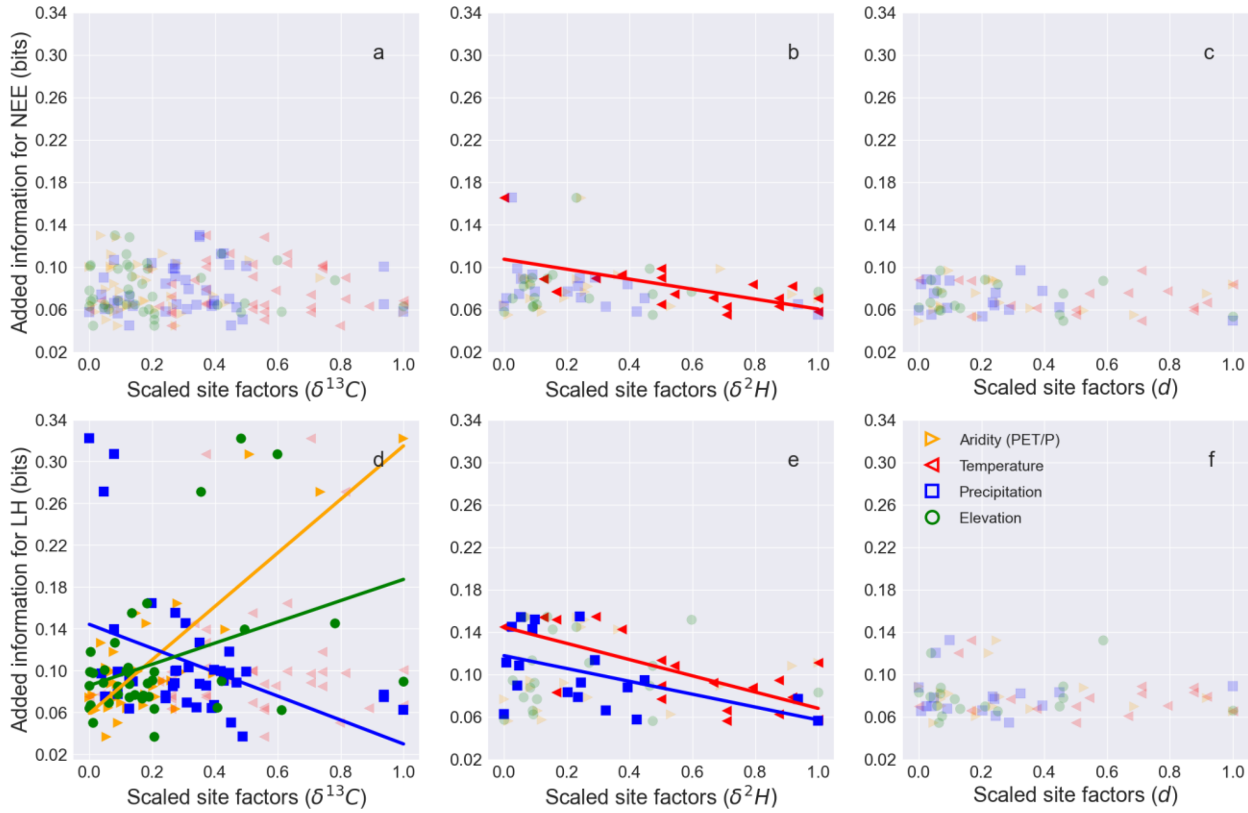

Figure 4 The total added information of $\delta^{13}C$ (a), $\delta^{2}H$ (b), and d (c) about net ecosystem exchange (*NEE*) against scaled site-specific variables. The total added information of $\delta^{13}C$ (d), $\delta^{2}H$ (e), and d (f) about latent heat flux (*LH*) against scaled site-specific variables. Solid lines indicate a significant p-values (< 0.05) of the slopes.