

Response to Reviewer 1:

Text from reviewer 1 is black, with our response in red, and added/edited text in the manuscript in blue.

Stable isotopes measured by the National Ecological Observatory Network (NEON) might provide unique information about terrestrial water and carbon exchanges. To drive this point home, Li et al. performed a formal information assessment to evaluate how $\delta^2\text{H}$, $\delta^{18}\text{O}$, and $\delta^{13}\text{C}$ can provide unique, synergistic, and redundant information about net ecosystem exchange (NEE) and latent heat (LH) and compared them with traditional meteorological data. The study will appeal to a broad audience interested in the carbon cycle, ecological modeling, and climate modeling. In summary, the paper should be accepted for publication pending minor revisions to enhance its conclusions.

Response: Thank you for your support of this study.

The main issue I have with this paper is the confusing data presentation in the figures. For example, in Fig. 1, what is the difference between the left, middle, and right columns? They have different labels only for the rightmost column, but the rest share the same labels. Furthermore, in Fig. 2, synergistic information, according to Eq. 3, requires X and Y in addition to Z (NEE or LH in this case). Why is the synergistic information label in the form of $S(X; Z)$ instead of $S(X, Y; Z)$? According to the paper, “synergistic information (S) [...] is the information provide (sic) to the Z when X and Y act jointly.” Can synergistic information be computed with X alone and without Y? Lastly, again in Fig. 2, to be consistent with Eq. 3, shouldn’t NEE and LH be the second parameter in the X-axis labels? In other words, NEE and LH are “Z” in Eq. 3 because the test is on the information isotopic and meteorological data can provide to NEE and LH. I am not an expert on formal information assessment, so maybe I am missing something here, but clearer labeling will make the paper more accessible to the broader audience.

Response: Following the reviewer’s suggestions, we remade the figure so that each information pair only shows up once based on resampling the data. The main difference between these columns in the prior figure was availability of the isotope data points. The resampling processes were done separately for each combination (i.e., resample [LH, NEE, T, VPD, R_g , u, isotope] individually). Therefore, the resampling process produces the nearly the same mutual information quantity but based on different isotope data availability. We therefore combined all the same quantity that is computed due to different isotope availability to a single box in the figure below.

We have remade figure 1 as following:

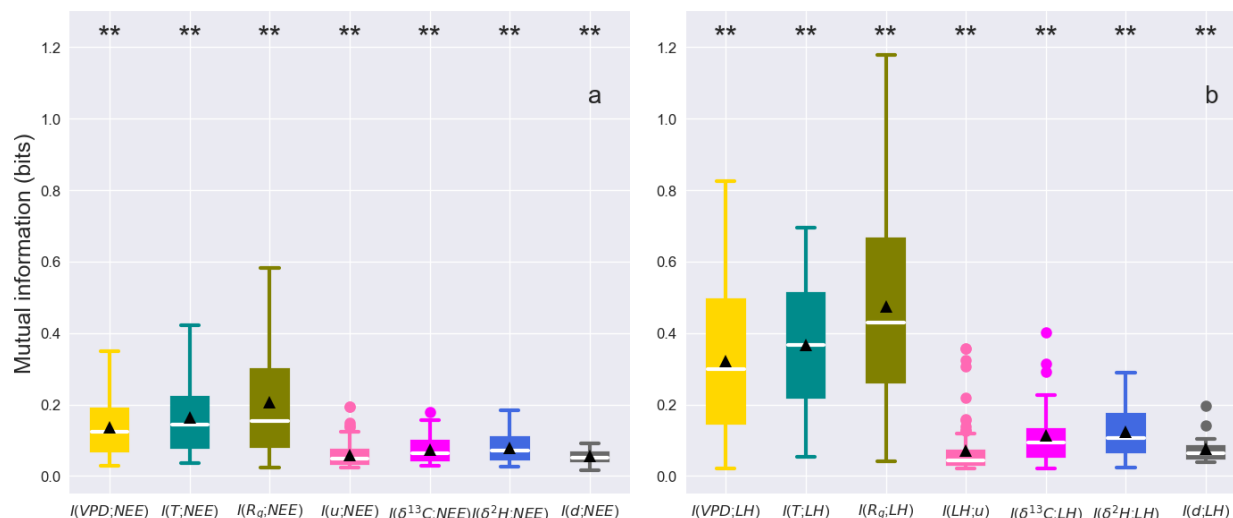


Figure 1 (a) Individual mutual information, $I(X;Y)$, shared between net ecosystem exchange, NEE , and each individual meteorological variable (vapor pressure deficit, VPD , air temperature, T , global radiation, R_g , windspeed, u). (b) Individual information shared between latent heat flux, LH , and each individual meteorological variable. Boxes of mutual information between meteorological variables and flux are consists of the same quantity that is calculated based on different isotope availability (e.g., box of $I(VPD; NEE)$ consists of $I(VPD; NEE)$ based on the availability of $\delta^{13}C$, $I(VPD; NEE)$ based on the availability of δ^2H , and $I(VPD; NEE)$ on the availability of d , collectively). 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).

We agree that synergistic information cannot be computed without X , Y , and Z and the label of synergistic information should be consistent with the equation in the manuscript. Following the suggestions of the reviewer we changed the label of figure 2 as the following.

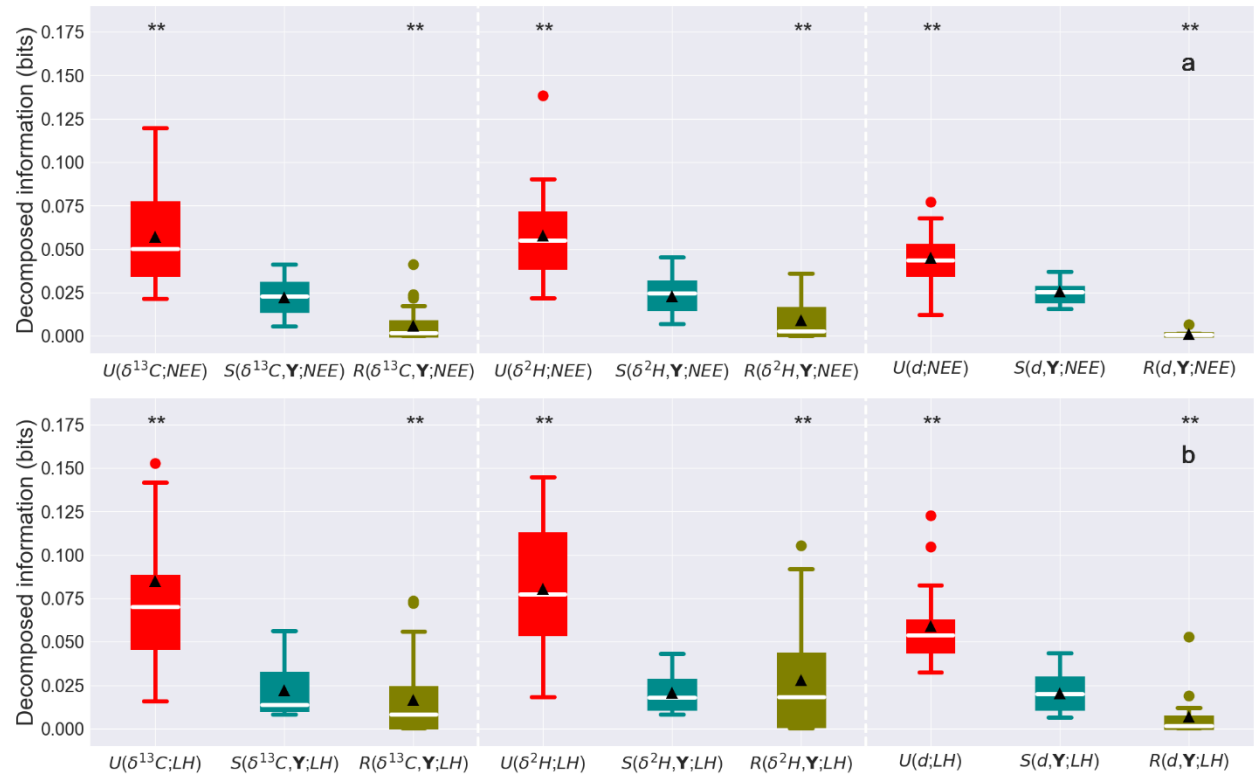


Figure 2 (a) The unique information, U , synergistic information, S , and redundant information, R , of the $\delta^{13}C$, δ^2H , and d stable isotope flux ratios on the net ecosystem exchange, NEE , and (b) latent heat flux, LH . The values of S , and R are calculated by averaging across different meteorological variables, indicated by Y (e.g., the average over $S(\delta^2H, VPD; LH)$, $S(\delta^2H, T; LH)$, $S(\delta^2H, u; LH)$, and $S(\delta^2H, R_g; LH)$ for S). 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).

We also changed the label of redundant information to $R(X, Y;Z)$ as it depends on both variables. We have also changed the labeling & notation across the manuscript. For instance, $I(NEE;VPD)$ was change to $I(VPD;NEE)$.

Additional minor suggestions for consideration:

P2L33 – The sentence “These results demonstrate ...” is hard to follow. Maybe break it up into multiple sentences.

Response: We have removed this sentence in the revised manuscript.

P2L47 – Remove “time domains.”

Response: We have removed these words as suggested.

P4L134 - I assume d is $\delta^{18}\text{O}$, but this is never explained. If that is the case, I would recommend just using $\delta^{18}\text{O}$ here and elsewhere in the text and in all the figures. The abbreviation doesn't save that much space and is confusing.

Response: We thank the reviewer for the comments. Indeed, the d refers to the deuterium excess. i.e., $d = \delta^2\text{H} - 8 * \delta^{18}\text{O}$. We have added the following to Line 117 “The $\delta^{18}\text{O}$ values were converted to deuterium excess (d) via $d = \delta^2\text{H} - 8 * \delta^{18}\text{O}$ (Dansgaard, 1964)” for clarification.
”

P5L145 - Here and elsewhere, remove “the” before “Z.”

Response: We have removed the word as suggested.

P5L145 – Change “provide” to “provided.”

Response: We have modified the word as suggested.

P6L197 – In this paragraph, the result presented in Fig. 3 is described. However, even though Fig. 3 consists of maps, the spatial distribution of the additional information is not discussed at all. Here or later in the Discussion, please add more text on the spatial variability.

Response: When discussing Fig 3, we added the following to Line 243 in the revised manuscript “ $\delta^{13}\text{C}$ contributes the most substantial information about NEE and LH in the Northeastern US (i.e., New Hampshire) and southwester US (i.e., New Mexico), respectively (Fig. 3a and Fig. 3d). In northern Alaska, $\delta^2\text{H}$ contributes the largest amount of additive information to NEE (Fig. 3b). There is an increased possibility of observing more additive information of $\delta^2\text{H}$ about LH at site with higher latitude (Fig. 3e). The highest additional that d provides to NEE and LH were observed in Virginia (Fig. 3c) and Wyoming (Fig. 3f), respectively.”

Regarding the spatial variability of Fig 3 in the Discussion, we have also added the following to Line 351 in the revised manuscript: “Variations in additional information across NEON sites indicate differences in conditional dependencies of ecosystem fluxes on processes related to isotope fluxes. Changes in ecosystem structure and climate affect the ecosystem's adaptability to environmental changes (Weiskopf et al., 2020) that influences the biochemical processes responsible for isotope fractionation, which can intensify or weaken these conditional dependencies.”

P6L201 – The reference to the figure panel is wrong. Change “Fig. 3a” to “Fig. 3d-f”.

Response: We thank the reviewer for this comment. We have revised as suggested.

P6L211 – The sentence “For these bulk fluxes, we showed ...” needs a reference to a figure so the readers know which data you are talking about.

Response: We thank the reviewer for this comment. We added Fig. 1 as a reference to this sentence.

P7L251 – Change “should be towards” to “should move towards.”

Response: We have changed the phrase as indicated.

P8L282 – This sentence has too many clauses and is hard to follow. Break it up into multiple sentences.

Response: We thank the review for this valuable comment. We have rephrased the referred sentence as “One of key motivations for measuring stable isotopes of water and carbon fluxes is that they may provide unique and novel knowledge about key mechanisms across ecosystems (Conrad et al., 2012; Good et al., 2014; Wang et al., 2010)Such hypothesis has not been formally tested until this study.”

References - Reference style is different from the journal convention. For example, there should be spaces between the first and middle name initials. There should be no period between the author names and the article title. The year should be between the author names and the article title.

Response: We have changed the citation style according to ERL’s citation convention.

SI P1L13 – Change “in most of cases” to either “in most cases” or “in most of the cases.”

Response: We have changed as suggested.

SI P2L41 – Change “significant test” to “significance test.”

Response: We have changed as suggested.

References

- Conrad, R., Klose, M., Yuan, Q., Lu, Y., & Chidthaisong, A. (2012). Stable carbon isotope fractionation, carbon flux partitioning and priming effects in anoxic soils during methanogenic degradation of straw and soil organic matter. *Soil Biology and Biochemistry*, 49, 193–199. <https://doi.org/10.1016/j.soilbio.2012.02.030>
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Response to Reviewer 2:

Text from reviewer 2 is black, with our response in red, and added/edited text in the manuscript in blue.

COMMENTS TO THE AUTHOR(S)

The research provides a compelling approach towards understanding the relationship between isotopic measurements and environmental fluxes. The use of information theory and partial information decomposition (PID) framework provides valuable insights into the amount of unique, synergistic, and redundant information provided by isotopes to environmental fluxes. The approach, particularly in analyzing the unique information contained within $\delta^{13}\text{C}$ and $\delta^2\text{H}$, provides a novel perspective for interpreting environmental fluxes. The manuscript is well-structured and addresses an important scientific question.

However, I have a few suggestions that might help to further strengthen this manuscript.

Response: Thank you for your support of this study.

Abstract

The abstract at present emphasizes the methodology and purpose but could be enhanced by a succinct, clear overview of the key results and implications of your study. A clear and concise summary of the main outcomes and their significance will capture the reader's attention more effectively.

Response: This is a good suggestion from the reviewer. We have revised the abstract to include the following “Overall, we show that the stable isotope datasets collected by NEON contribute non-trivial amounts of new information about bulk environmental fluxes useful for interpreting biogeochemical and ecohydrological processes at landscape scales. However, the utility of this new information varies with environmental conditions at continental scales. This study provides an approach for quantifying the value adding non-traditional sensing approaches to environmental monitoring sites and the patterns identified here are expected to aid in modeling and data interpretation efforts focused on constraining carbon and water cycles’ mechanisms.”

Methods

The decision to use mutual information (MI) and unique contribution (UC) as measures of the information provided by isotopes and other variables is clearly outlined. It would be beneficial, however, to provide further explanation or rationale for choosing these specific measures to improve the understanding of readers who might not be as familiar with these concepts.

Response: We thank the reviewer for this comment.

We added “In this study the mutual information metric, $I(X;Y)$, was chosen to analyze how different meteorological variables share information about ecosystem fluxes because it has the advantage over traditional metric (e.g., correlation coefficient) of capturing both linear and non-linear dependencies between two variables. It represents the reduction in uncertainties of one variable given the knowledge of another variable.” to Line142 in section **2.2 Information measures**.

We also added “This framework captures how the different source variables interactively influence a target variable of interest, which can possibly reveal the process that relates source variables and a target without any modeling assumptions.” to Line 173 in section 2.3 Partial information decomposition.

Results

The results section provides a wealth of insightful information. Nonetheless, it might be worth discussing the potential reasons for the variability in the unique information provided by isotopes across different sites, climates, and ecosystems. Providing more context or hypotheses for these observed differences would be informative.

Response: We thank the reviewer for this comment. We have provided some text about variability in unique information text (Please also refer to response of 3 and 4 of Discussion) in the 4. Discussion. Since the key results of the study are the information qualities, we chose to keep the discussion of factors driving these values in the discussion.

Discussion

1. Dataset description. While the methods provide a detailed breakdown of the mutual information calculation and the PID framework, a clearer summary of the datasets used would be beneficial. The authors have referred to the Supplemental Information for more details, which is acceptable; however, providing a concise summary within the main manuscript might add clarity for readers. Then, go into full details in the Supplemental Information.

Response: We thank the reviewer for this comment. We have added the following paragraph “The *NEE* and *LH* data were filtered for periods of low turbulence based on friction velocities (u^*) then gap-filled using the marginal distribution sampling method (Wutzler et al., 2018). The gap-filled and u^* filtered 30-minute fluxes were further averaged on a daily scale to facilitate future analysis. All 30-minute meteorological variables except wind speed were gap-filled using the marginal distribution sampling mentioned above. The gap-filled meteorological variables were then averaged to daily scale. Extreme values in daily flux and meteorological datasets were further processed using an inter-quantile filter (Goodwell & Kumar, 2017).” to Line 126 in 2.1 Study sites and data preparations.

2. Clarity. While the authors discuss the unique information provided by isotope ratios in detail, some sections might be difficult to understand for readers not deeply familiar with the subject. It might be beneficial to present this information in a more accessible way, considering the general readership of ERL (as opposed to, for example, IEEE Transactions on Information Theory), possibly by using more layman's terms or by including a brief recap of the fundamentals. For example, the use of mutual information (MI) and unique contribution (UC) as measures of information provided by isotopes and other variables was clearly stated. However, a detailed explanation of the decision to use these specific metrics might provide better context for readers who are not as familiar with these measurements. If the authors are constrained by the length limits in the main text, then they should make full use of the Supplemental to discuss these in detail.

Response: We thank the reviewer for the comment. The recap the fundamentals of these information quantity, we have added some text following text “This formally demonstrates that *NEE* and *LH* become

less uncertain given the knowledge of isotope data or meteorological data throughout the NEON sites.” to Line 197 in **3. Results**. The following text “(i.e., the information contribution that is contributed only by one variable to the target variable)” was added to Line 224 in **3. Results**. The following text “(i.e., the information component when isotope and other variables act jointly to provide information about ecosystem fluxes)” was added to Line 233 in **3. Results**. “(i.e., the overlapping information that isotope or other variables contribute to ecosystem fluxes)” was added to Line 233 in **3. Results**. The decisions of why these metrics were used were given at methodology. Please also refer to response under “Methods” above.

3. Site-specific considerations. The authors discuss the impact of site-specific conditions (e.g., aridity, precipitation) on the unique information provided by isotopes. However, it would be useful to elaborate on the specifics of these conditions. For example, under what conditions do isotopes provide the most (or least) unique information? Are there any other site-specific considerations that were not included in the study? Moreover, the conditions are evidently ‘atmospheric science centric’. How about the subsurface conditions (e.g., depth to water table, slope, aspect, etc.) and porous media properties that also drive LH and NEE? Are these also not measured at (some if not all) NEON sites? Not ignoring the dynamics belowground and geomorphic variables would at least be a fair characterization of the complexity of the system that the work has undertaken to describe within the framework of information theory.

Response: We thank the reviewer for this comment. Indeed, the relationship between the unique information of isotopes to ecosystem fluxes and site-specific conditions are quite similar to what has shown on Figure 4 of the manuscript because the total additive information is dominated by the unique information. We added the following text “There is a higher chance that $\delta^{13}\text{C}$ contributes more information about *LH* under drier conditions or lower precipitation conditions (Supplemental Fig. S4). Additionally, both $\delta^{13}\text{C}$ and $\delta^2\text{H}$ tend to provide more distinct insights into *NEE* and *LH* in cooler or lower precipitation conditions.” to Lin 318 in **4. Discussion**. We also added a new figure to the supplementary material (Supplemental Fig. S4, below).

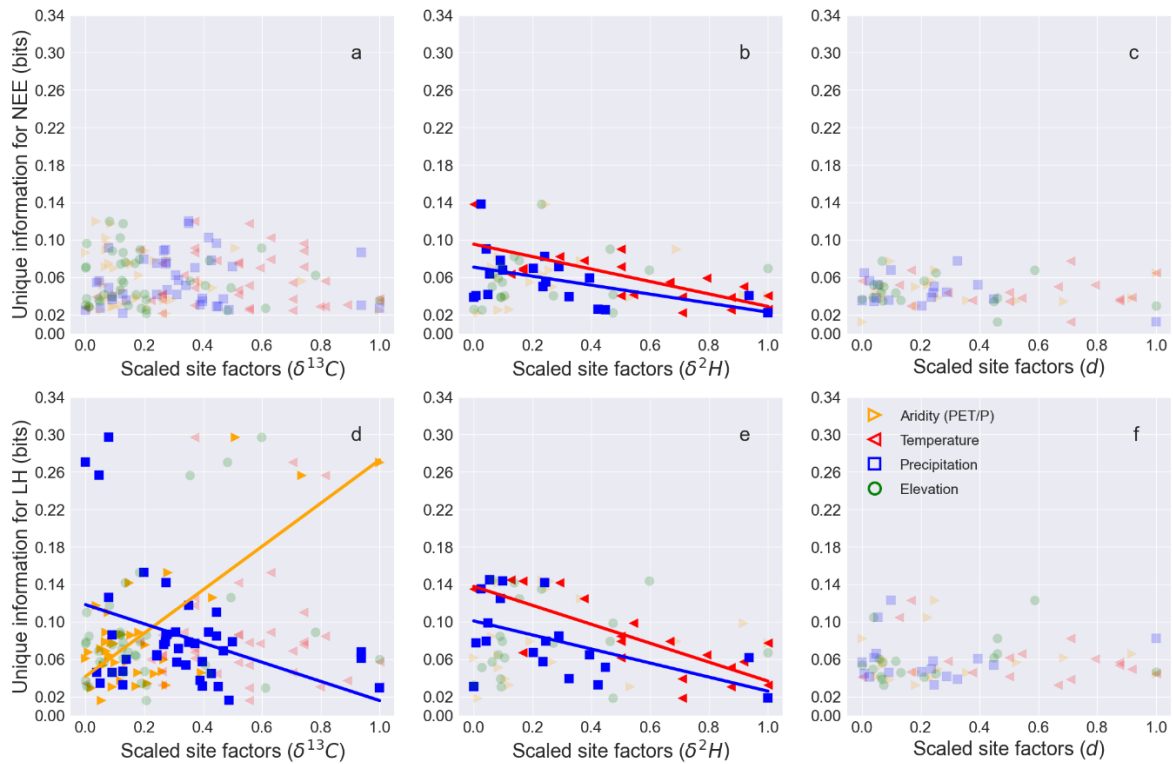


Figure S4 The unique information of $\delta^{13}\text{C}$ (a), $\delta^2\text{H}$ (b), and d (c) about net ecosystem exchange (NEE) against scaled site-specific variables. The unique information of $\delta^{13}\text{C}$ (d), $\delta^2\text{H}$ (e), and d (f) about latent heat flux (LH) against scaled site-specific variables. Solid lines indicate a significant p -values (< 0.05) of the slopes.

We also acknowledge as a caveat that we primarily consider factors that are atmospheric science centric, and we did not consider other site characteristics such as vegetation (rooting depth, biomass density), soil (soil types, saturated hydraulic conductivity), and subsurface conditions (water table depth).

Therefore, we have added “It’s worth noting that this study primarily explored how each isotope contributes additional information to NEE and LH with an emphasis on atmospheric centric conditions. However, it is crucial to acknowledge that ecosystems broadly have a wide range of complexities, , such as geomorphology (e.g., slope, aspect) subsurface dynamics (e.g., depth to water table), vegetation species and traits (e.g. plant hydraulic traits), and soil physics (e.g., soil texture), which might play a role in shaping the way of how isotope observations provide extra information about NEE and LH .” to Line 356 in 4.Discussion

4. Methodological considerations. The authors mention that the additional information provided by isotopes may vary across sites, climate, and ecosystems. It would be informative to elaborate on why this variation might occur and how it was handled in the methodology in this study.

Response: We thank the reviewer for the valuable comment. The following sentence has been added to Line 351 in 4. Discussion to address the reviewer’s concern. “Variations in additional information across NEON sites indicate differences in conditional dependencies of ecosystem fluxes on processes related to isotope fluxes. Changes in ecosystem structure and climate affect the ecosystem’s adaptability to environmental changes (Weiskopf et al 2020) that influences the biochemical processes responsible for

isotope fractionation, which can intensify or weaken these conditional dependencies.” In order to handle this such variation, we treated all data points equally. In the methodology, we were careful to devise the resampling approach so that the same number of datapoints was used from each site.

5. Future research directions. While the authors suggest investigating how the results might vary with more available datasets and a wider range of environmental conditions, it would be valuable to expand on the potential directions for future research. Are there any specific conditions, variables, or models that should be explored in the future? Providing specific examples of the conditions, variables, or models that should be explored in the future will offer readers a clear direction for subsequent research. At present, it is almost impossible to appreciate how other researchers can make use of the results of this study, for example, in various possible applications in earth and environmental sciences.

Response: We thank the reviewer for this comment. The following paragraph was added to Line 378 “It is important to acknowledge that our analysis focused on how daily isotope datasets are informative of bulk ecosystem fluxes. It might be worthwhile to analyze how similar observations are informative of ecosystem fluxes at finer temporal scales. For instance, how lags in isotope dataset responses are influenced ecosystem processes, and correspondingly how do the partial information components change with different lag timescales can possibly reveal more detailed linkages between ecosystem fluxes and isotope fluxes. In this study, we considered abiotic variables (VPD , T , u , R_g) as the confounding part in the partial information decomposition. It might also be worthwhile to explore how other biotic variables such as ecosystem structure, species composition, and plant hydraulic traits, rooting depth can influence the total additive information of isotope dataset to the bulk fluxes.”

6. Inclusion of isotope flux ratios in models. The authors conclude by suggesting that their results could guide the improvement of model results after the incorporation of isotope flux ratios. It would be valuable to detail what specific improvements they expect or suggest and to discuss potential challenges or considerations for this incorporation.

Response: We appreciate the reviewer for this valuable comment. We added the following text to Line in 329 **4. Discussions** “The incorporation of isotope datasets into artificial intelligence (AI) and machine learning (ML) models, especially explainable AI models, can potentially improve predictive accuracies and enhance our understanding of ecosystem fluxes. Nevertheless, uncertainties can be introduced when incorporating isotope dataset to models with larger spatial scale. It is challenging to include isotope datasets to models that require larger spatial scale isotope datasets, as they are often hard to acquire. Researchers might also consider different incorporation strategies in different ecoclimate regions.”

7. δ^2H vs. $\delta^{18}O$. There is a preponderance of mention of δ^2H . How about $\delta^{18}O$? The last mention of $\delta^{18}O$ is in L93. The rest of the manuscript focused solely on δ^2H .

Response: We thank the reviewer for his comment. We converted $\delta^{18}O$ to deuterium excess. We have added “The $\delta^{18}O$ values were converted to deuterium excess (d) via $\delta^2H - 8 * \delta^{18}O$ (Dansgaard, 1964b)”

8. Physical basis for results. L174-176. What is the physical basis or explanation for this result? (Instead of $\delta^{13}C$ values best constraining NEE and δ^2H or d values best constraining LH, we find that δ^2H values on average provide slightly more mutual information than $\delta^{13}C$ values for both NEE and LH fluxes....) It is

one thing to that these results are ‘highly unlikely to be obtained by random processes’ (L178-179), but what is the physical basis? In the book, The Physics of Information Technology, Neil Gershenfeld argued the connection between information theory (bits, i.e., the fundamental unit anchoring this manuscript in review) and physics. At the least, the authors are encouraged to explain the physical basis for this result, because quite frankly, this result (L174-176) does not make physical sense at all.

Response: We thank the reviewer for this comment. We have provided the following sentences to Line 213 in **3. Results** for explanation. “*NEE* is a quantity that encompasses downward carbon uptake via plant photosynthesis and carbon release upward through respiration (Reichstein et al., 2005) while water, as represented by *LH*, is evaporated upward during evapotranspiration. δ^2H links with the phase transformation of water that is strongly temperature dependent (Xiao et al., 2018). Therefore, δ^2H is more likely to carry slightly more information about *LE* and *NEE* than $\delta^{13}C$.”

Minor comments

L33-35. This sentence seems off or that a word or phrase must be missing. Please rewrite for clarity.

Response: We thank the reviewer for this comment. We have removed this sentence from the abstract.

L73. Subject-verb agreement. Please rewrite.

Response: We have rephrased “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” to “Previous network-based studies of δ^2H , $\delta^{18}O$ and $\delta^{13}C$ examined patterns across distinct ecosystems using cryogenic baths and flask samples; however, the poor temporal sampling and spatial coverage has limited these approaches to understand ecosystem-scale processes (Gemery et al., 1996; Orlowski et al., 2018).”

L113. Typos 30-minte and gap-filling.

Response: We thank the reviewer for this comment.

L134. What’s *d*? deuterium excess? This apparently important variable just came out of nowhere.

Response: We added “The $\delta^{18}O$ values were converted to deuterium excess (*d*) via $\delta^2H - 8 * \delta^{18}O$ (Dansgaard, 1964).” to Line 138 in **2.1 Study sites and data preparations**.

L145. Typo provide

Response: We thank the reviewer for pointing out this typo. We have corrected it.

L264. Typo demonstrate.

Response: We have corrected this typo.

L288. Typo dominate.

Response: We have corrected this typo.

References

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