Authors Response to Reviewer 1 Comments for Manuscript egusphere-2024-4163: *The primacy of dissolved organic matter to aquatic light variability*

9 May 2025

The authors thank Reviewer 1 for their valuable comments. The authors respond to all comments below and document resulting modifications to the manuscript, as appropriate. Reviewer 1's comments are shown in *slanted* typeface. The Authors responses are shown in plain typeface. Revised or added text is indicated in red. All line numbers are indicated with a capital "L" and refer to the line numbers in the original submitted work. Citations within this response document correspond to the References section at the end of this document.

- **Comments from Reviewer 1:** *The manuscript by Houskeeper and Hooker presents a novel perspective on the primacy of colored dissolved organic matter (CDOM) over chlorophyll a (C_a) in driving aquatic light variability. This manuscript makes a significant contribution to the field of ocean optics by challenging long-standing assumptions about the primacy of C_a in driving aquatic light variability. Their comprehensive analysis of three independent bio-optical datasets provides compelling evidence that CDOM absorption—not C_a—represents the dominant factor influencing spectral variability in aquatic environments. This finding has profound implications for ocean color remote sensing, potentially reshaping algorithm development and improving our ability to monitor marine ecosystems from space. The authors' demonstration that expanded spectral ranges (including UV and NIR domains) improve the independent retrieval of optical constituents provides timely insights for utilizing data from new hyperspectral satellite missions like PACE. Their work effectively bridges historical perspectives on ocean optics with contemporary understanding of microbial loop dynamics, offering a more nuanced view of the biogeochemical processes influencing marine optical properties. Overall, the paper represents a valuable contribution that could significantly advance our ability to interpret and utilize ocean color observations in a changing climate.*

  Authors Response 1: The authors thank the reviewer for the positive comments.

  While their eigendecomposition analysis is thorough, I have concerns about terminology and methodology. The authors repeatedly refer to "EMA" (end-member analysis) without adequately explaining this approach or its relation to established methodologies. Have they invented it? If so, I am not sure it warrants a name nor acronym.

  Authors Response 2: End-member analysis (EMA) is an algorithmic approach wherein information is captured from the most spectrally separated (e.g., ultraviolet, UV, and near-infrared, NIR)—rather than from the internal (primarily VIS)—wavelengths. The concept was first described in Hooker et al. (2013) and the terminology was introduced in Hooker et al. (2020), which also noted that this approach provides continuity between historical multispectral observations and forthcoming hyperspectral observations:

> "... the simplified approach provided by end-member analysis can be used with both legacy and next-generation sensors, thereby providing continuity in space and time as well as a capability to generate high-quality in-water data with a simplified measurement approach..."

The EMA approach was subsequently leveraged to develop aquatic remote sensing algorithms or investigate optical relationships in Houskeeper et al. (2021,2022) and Hooker et al. (2021a,b). Greater community adoption—and therefore familiarity—with EMA is, perhaps, limited by the sparsity of compliant UV and NIR aquatic radiometric datasets.

The authors clarify this topic by better defining EMA at its first usage (L016–017), as follows:

> "... based on using ratios of the most spectrally separated optical data products (Hooker et al. 2013), especially those from the UV and NIR spectral domain, an approach hereafter termed end-member analysis (EMA) following Hooker et al. (2020). Conservative waters..."

After investigating their cited works and testing their CDOM prescription against the Loisel et al. (2023) dataset (see: `https://github.com/ocean-colour/bing/blob/ema/nb/EMA/Explore_EMA.ipynb`*), I found their approach exhibits sensitivity to algorithm variants that warrants further discussion. The authors appear to have developed this method across several publications, but it requires more explicit contextualization for readers unfamiliar with their previous work, particularly regarding how different implementations might affect results.*

Authors Response 3: The authors revise elements of the manuscript to provide context based on the reviewer's point. But first, some clarifications are warranted regarding the reviewer's referenced Python notebook.

Briefly, the reviewer has attached a notebook using data wherein synthetic apparent optical properties (AOPs), e.g., $\left[L_W(\lambda)\right]_{\mathrm{N}}$, are synthesized from various datasets of inherent optical properties (IOPs), e.g., $a_{\mathrm{CDOM}}(440)$. For individual AOP observations in this dataset, the suite of IOPs needed to derive the AOP do not represent the same set of *in situ* observations, i.e., they include dissimilar sampling times or locations. IOPs are randomly assembled using each IOP's distribution, and from these random assemblages, AOPs such as $\left[L_W(\lambda)\right]_{\mathrm{N}}$ are derived. The synthetic dataset, therefore, is not constrained to the associations that exist among *in situ* IOPs in the ocean (Morel 2009) or aquatic environments.

Conversely, the applicable algorithm from Houskeeper et al. (2021), i.e., GLOBC, was derived using *in situ* observations of aquatic environments. GLOBC thereby includes *in situ* relationships in IOPs—generally discussed in terms of optically active constituents (OACs) in the manuscript under review.

The reviewer's notebook tests the performance of EMA algorithms using both the applicable tuning (GLOBC), as well as two inapplicable tunings (OCEAN and NOMAD). The latter correspond to observations derived using legacy above- and in-water instrumentation, with in-water data products derived in a deep extrapolation column with coarse vertical sampling resolution (VSR), and above-water data products derived using slow sampling speeds (on the order of 0.5 Hz) and low signal-to-noise ratio (SNR) observations (Kudela et al. 2024).

The reviewer's notebook graphic shows two characteristics, both of which the authors consider to be consistent (not inconsistent) with the published literature:

1. The reviewer's graphic shows that synthetic data products produce increased scatter and nonlinearity compared to *in situ* data products. This finding is anticipated and consistent with the literature, as follows: random re-organization of IOPs removes the OAC covariances observed within *in situ* water bodies; removing OAC covariances increases variability in OACs; and increasing variability in OAC relationships increases scatter in visible (VIS) algorithms.

   Algorithm sensitivity to variability in OACs was shown to be a function of algorithmic spectral range, which was the primary finding of Houskeeper et al. (2021). Non-visible—or invisible (INV)—algorithms are more robust to OAC variability than VIS algorithms. The reviewer's notebook implements VIS algorithms and has shown, as is expected, that removing IOP or OAC covariances increases the scatter for VIS algorithms.

   For example, consider this text from Houskeeper et al. (2020):

   > "…correlation to $a_{\mathrm{CDOM}}(440)$ increase[s] with greater spectral separation of the waveband ratio toward ultraviolet and near-infrared wavelengths."

   Another example, from Houskeeper et al. (2021):

   > "For all datasets, the dynamic range in [the waveband ratio] increases with increasing spectral separation between wavelength pairs, which is anticipated to increase the sensitivity and robustness of the algorithmic approach."

   And another, from the submitted manuscript (L445–447):

   > "Linearity and loglinearity of CDOM algorithms decreases with decreasing spectral separation of algorithm end members (Hooker et al. 2020, 2021a; Houskeeper et al. 2021) because increasing overlap in OAC absorption properties adds nonlinearity (Houskeeper et al. 2020a)."

Regarding relationships among OACs, the observed covariances within *in situ* water bodies have been fundamental to the development of ocean color algorithms, namely the Ocean Chlorophyll (OC) family of algorithms. The authors' manuscript does not argue against the existence of covariances among OACs within oceanic and global *in situ* data products, which are well documented (Morel et al. 2009; Hooker et al. 2021a). Rather, the authors have previously shown that EMA algorithms—especially INV but also VIS implementations—mitigate some of the algorithmic sensitivity to variability in the OAC relationships.

Finally, the scatter in the notebook graphic for the applicable algorithm (GLOBC) appears to be consistent with the uncertainty reported in Houskeeper et al. (2021) for the VIS algorithm, i.e., 45% (although uncertainty metrics are not presented in the graphic).

2. The reviewer's graphic shows that algorithms become biased if retuned using legacy data products (i.e., the OCEAN and NOMAD tunings), which are often nonphysical, e.g., negative or signal limited, and biased. The authors strongly agree and have discussed this challenge in many contexts (Hooker et al. 2020, 2021a, 2021b; Houskeeper et al. 2020, 2021, 2023, 2024; and Kudela et al. 2019, 2024). The reviewer's graphic provides additional support for this trajectory of literature by showing that algorithms derived using legacy AOP data products (most notably those of NOMAD) are strongly biased compared to AOP data products synthesized using radiative transfer. The point is consistent with the submitted manuscript, which did not use NOMAD data products based, in part, on the previously published findings indicating bias.

The authors revise the text to help clarify elements related to implementation of the EMA algorithms.

First, the authors clarify the tuning (to avoid readers implementing the OCEAN or NOMAD coefficients from the Python notebook) by specifying the applicable coefficients directly in Eq. 2, as follows:

$$a_{\mathrm{CDOM}}(440) \;=\; 0.242 \left[\Lambda_{\lambda_2}^{\lambda_1}\right]^{-0.961}, \qquad [\mathrm{m}^{-1}] \tag{1}$$

The authors add discussion regarding decreased performance of VIS implementations compared to INV implementations at L113, as follows:

> "...indicating the importance of accurately deriving UV data products for robust CDOM estimation. VIS algorithms, conversely, were shown to exhibit decreased robustness to variability in OAC relationships relative to INV algorithms (Hooker et al. 2020, 2021b; Houskeeper et al. 2020, 2021).

The authors revise text on L601–603 to clarify EMA is leveraged herein is improved robustness to OAC relationships, and the improvement is dependent on the spectral range (e.g., VIS compared to INV), as follows:

> "Spectrally expansive data products have been shown to improve retrieval of $a_{\mathrm{CDOM}}(440)$ independent of C_a (Sathyendranath et al. 1987; Hooker et al. 2020; Houskeeper et al. 2021), attributed, in part, to improved robustness to variability in the relationships between OACs. The comparisons herein of eigenanalyses using the INV21 and VIS21 spectral subsets further support the hypothesis that an expansive spectral range for data products improves the separability of signals.

The authors improve discussion of the limitations by adding text regarding the efficacy of EMA when applied to legacy datasets (wherein spectral range is generally confined to VIS wavelengths). Most notably, the RSE2022 dataset corresponds to much coarser VSR plus depth aliasing (see L215–217 of the manuscript) and commercial-off-the-shelf (COTS) spectrometers limiting the SNR (Kudela et al. 2019; 2024). The authors add text to L265, as follows:

> "The uncertainty of EMA is anticipated to increase when applied to optical data products obtained using spectrometers and rocket-shaped profilers (e.g., RSE2022) due to increasing extrapolation depths combined with the strong attenuation of signal, particularly within the end-member spectral domains (Kudela et al. 2019, 2024; Hooker et al. 2020; Houskeeper et al. 2021)."

Deficient data quality (most applicable to RSE2022 which corresponds to degraded SNR and VSR) is presently managed, in part, by applying quality control metrics to identify and remove spectra that are likely nonphysical. For example, oceanic spectra that are significantly darker than the darkest global waters (as observed using much higher SNR and finer VSR technologies) are associated with SNR-limited measurements or depth aliasing within vertical profiles. The authors add discussion of sensitivity testing regarding quality control to L238, as follows:

> "…the threshold removal of nonphysical radiometric brightness was thus applied, albeit only using VIS data products (given that RSE2007 and RSE2022 are restricted to the VIS domain), following sensitivity testing. Briefly, more stringent quality control metrics (e.g., requiring observations to comply with the brightness ranges of the globally representative RSE2021 dataset) produced similar eigenanalyses results but reduced the size of RSE2022 by approximately 50%. Alternately, relaxed quality control thresholds permitting radiometric values up to 50 times darker than the global dataset did not alter the primary findings of RSE2022, and no threshold relaxation affected the primary findings of RSE2007. Considering acknowledged uncertainties relating to hardware, processing, data acquisition, and water mass differences, the quality control thresholds were performed within this insensitivity range by…"

The manuscript notably omits sufficient discussion of detrital absorption, which significantly contributes to absorption at wavelengths below 500nm. The authors acknowledge overlapping spectral characteristics between Ca and CDOM but don't adequately address how detrital absorption might influence their conclusions about CDOM primacy. Given that detritus can substantially affect spectral signatures in the same regions they analyze, this omission represents a gap in their analysis framework. A more comprehensive treatment of all optically active constituents would strengthen their argument regarding the relative importance of CDOM in aquatic environments.

Authors Response 4: The authors have not chosen to omit detritus or any other OAC from their study, but rather the analyses reflect the reality that detrital measurements are more sparse for globally applicable bio-optical datasets. Nonetheless, elements of the results describe detrital absorption, as follows: the leading eigenfunction for each dataset—the eigenfunction with a spectral shape most similar to that of detrital (but also CDOM) absorption—captures approximately 60% of the variance in each dataset. The datasets represent dissimilar water body types—ranging from purely oceanic waters (RSE2007) to oceanic, coastal, and inland waters in nearly equal representation (RSE2021). Contributions from detritus would therefore be anticipated to vary greatly between datasets. Differences in the variance captured between the datasets, however, are negligible (within ±1%), thereby not supporting strong differences in detrital effects. This means that although detritus certainly contributes to blue absorption in the dataset, the spectral modifications captured by the leading eigenfunction do not support primacy of detrital absorption. This point is also supported by the leading eigenfunction indicating strong linearly correlation to $a_{\mathrm{CDOM}}(440)$. Detrital absorption and CDOM absorption exhibit variable correlation for different natural waters (Babin et al. 2003; Twardowski et al. 2004), which would degrade the linear correlation if detritus was playing a major role in the analysis.

Therefore, the sparsity of detrital absorption data is unfortunate (and not due to omission by the authors), but the data and analyses nonetheless still support the findings presented. The authors improve discussion of detrital absorption by adding a new paragraph discussing detrital absorption following L467, as follows:

> "Observations of detrital absorption were not available, and detritus and CDOM share similarities in the spectral-shape of absorption, i.e., absorption increases for both at shorter wavelengths. Some key factors relevant to the focus herein on $a_{\mathrm{CDOM}}(440)$ over detritus in driving variability in aquatic spectra include that the leading eigenfunction captures similarly high proportions of the variance for each dataset (within 1% to the mean), whereas each dataset corresponds to dissimilar contributions from open-ocean waters. Absorption by CDOM and detritus also exhibit variable correlation patterns (Babin et al. 2003; Twardowski et al. 2004), which would degrade the correlation between the leading eigenfunction and $a_{\mathrm{CDOM}}(440)$, if the leading eigenfunction was strongly associated with detritus."

In addition, the authors add discussion of the benefits conferred by expanded field sampling, namely for detrital absorption and non-algal particles, at L515 (further discussed in Authors Response 25), as follows:

> "The findings demonstrate high variance captured by the leading eigenfunction and the eigenfunction's strong association with $a_{\mathrm{CDOM}}(440)$ variability, but the findings would be strengthened by adding field sampling for additional biochemical or bio-optical parameters. For example, RSE2021 demonstrates the importance of combining spectrally expansive radiometry and observations of C_a with observations of $a_{\mathrm{CDOM}}(440)$. Also adding observations of non-algal particles (NAPs) and detrital absorption would help to further improve clarity on the eigenfunction interpretations, and, perhaps, contribute to a better understanding of the subsequent modes."

Throughout the manuscript, the authors consistently refer to their analysis as an "eigendecomposition" rather than using more widely recognized terms like Principal Component Analysis (PCA) or Empirical Orthogonal Functions (EOF). While technically correct, this terminological choice may unnecessarily distance their work from the broader scientific literature, potentially impeding recognition of their method's relation to established techniques.

Authors Response 5: The authors improve clarity based on the reviewer's comment in two ways. First, when the eigenanalysis is introduced on L13, the authors add the terms "Empirical Orthogonal Function (EOF)" and "Principal Component Analysis (PCA)," as follows:

> "...is tested herein using eigenanalysis—e.g., an Empirical Orthogonal Function (EOF) analysis, Principal Component Analysis (PCA), or other eigendecomposition depending on the literature—on three independent bio-optical datasets ..."

Second, the authors replace the term "eigendecomposition" with the term "eigenanalysis" when it appears in the methodological description on L267–269 and the results text on L301.

Additionally, the manuscript would benefit significantly from showing the mean spectra alongside their eigenfunctions, as well as demonstrating reconstructed spectra with varying CDOM and Ca concentrations to illustrate how these constituents individually contribute to spectral variability.

Authors Response 6: Fig. A1 shows mean spectra plus reconstructed spectra based on varying influences of the eigenfunctions (the eigenfunctions are already shown in Fig. 1). The magnitude to which the reconstructed spectra are modified by the eigenfunctions (i.e., represented by the scalar in the legend) is selected based on the approximate inverse of the y-axis range in Fig. 1. That range is a mathematical consequence of the spectral resolution of each dataset and is not prescribed by the authors.

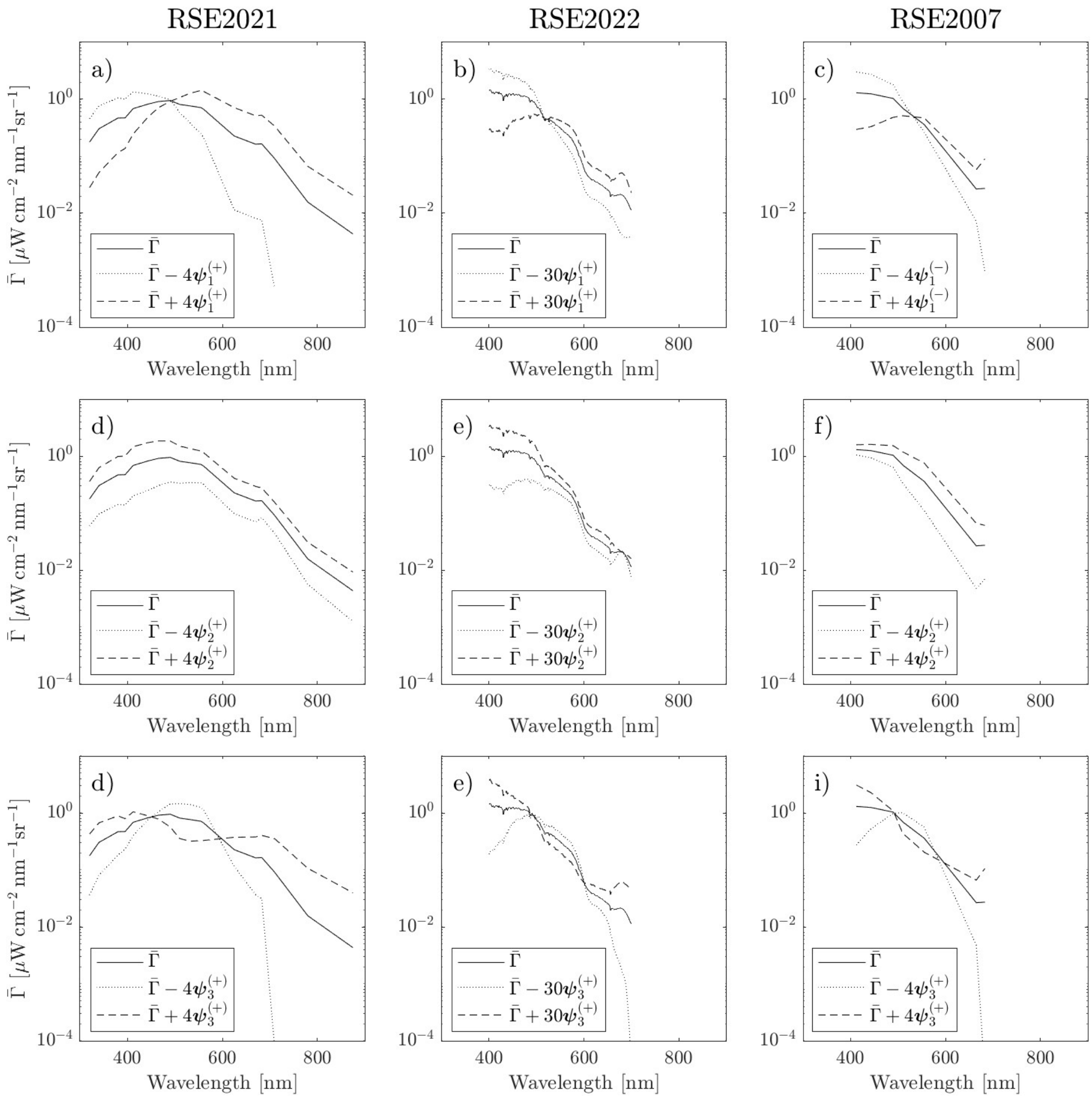

Fig. A1. Mean $\left[L_W(\lambda)\right]_{\mathrm{N}}$ spectra—represented as $\bar{\Gamma}$ for brevity following Hooker et al. 2021a—are shown for each dataset as solid black lines. Reconstructed spectra are shown in dashed plus dotted lines and represent spectral modifications associated with adding or subtracting, respectively, scalar quantities derived from the eigenfunctions. Modifications associated with $\boldsymbol{\psi}_1$, $\boldsymbol{\psi}_2$, and $\boldsymbol{\psi}_3$ are shown in the top, middle, and bottom rows, respectively.

The authors should acknowledge that their eigendecomposition approach assumes linear relationships among spectral variables, which may not fully capture nonlinear aspects of aquatic optical properties. Ocean color properties often exhibit complex nonlinear relationships, particularly in optically complex waters. This impacts some of the conclusions drawn. In particular, on Line 503-505, the authors write: "…the leading eigenfunction would be anticipated to capture nearly all of the variance of the dataset." This only holds if the relationships are linear.

Authors Response 7: The authors agree with the reviewer that eigenanalyses capture variability expressed in a linear framework. The authors also agree with the reviewer that ocean color properties can exhibit nonlinear relationships, while simultaneously acknowledging that quasi-linear approximations have been applied for decades. For example, Gordon et al. (1988) established a fundamental framework for relating IOPs to the remote-sensing reflectance, R_{rs}, wherein R_{rs} is proportional to the ratio of backscattering to absorption. In waters where absorption greatly exceeds backscattering (which include most global waters if considering VIS optical properties and nearly all global waters if considering INV optical properties), this fundamental framework would invoke approximately log-linear relationships, e.g., $\ln(R_{rs}) \propto -\ln(a)$. The authors also agree that nonlinearities, e.g., those commonly associated within case-1 algorithms wherein optical properties are empirically tuned to C_a (Morel et al. 2009), are applicable to the discussion of the idealized case-1 dataset at L503–505.

The analyses conducted herein do not negate nonlinear processes, but the datasets also do not suggest the eigenanalysis results are strongly swayed by nonlinearity. For example, the leading eigenfunction—which captures most of the variance for each dataset—produces $\boldsymbol{S}_1$ values with a distribution similar to that of $a_{\mathrm{CDOM}}(440)$. The $\boldsymbol{S}_1$ matrix predictors produce linear correlation to log-transformed $a_{\mathrm{CDOM}}(440)$ with Pearson's correlation coefficient indicated as ρ, plus Spearman's rank correlation coefficient included as $\tilde{\rho}$. High variance captured by the leading eigenfunction combined with loglinear relationships produced between $\boldsymbol{S}_1$ and a physically interpretable environmental parameter, support that the eigenanalysis is uncovering a dominant parameter influence, as intended. The relationships between the $\boldsymbol{S}_1$ plus $\boldsymbol{S}_2$ matrix predictors and $a_{\mathrm{CDOM}}(440)$ plus C_a, respectively, are shown in Fig. A2, as follows:

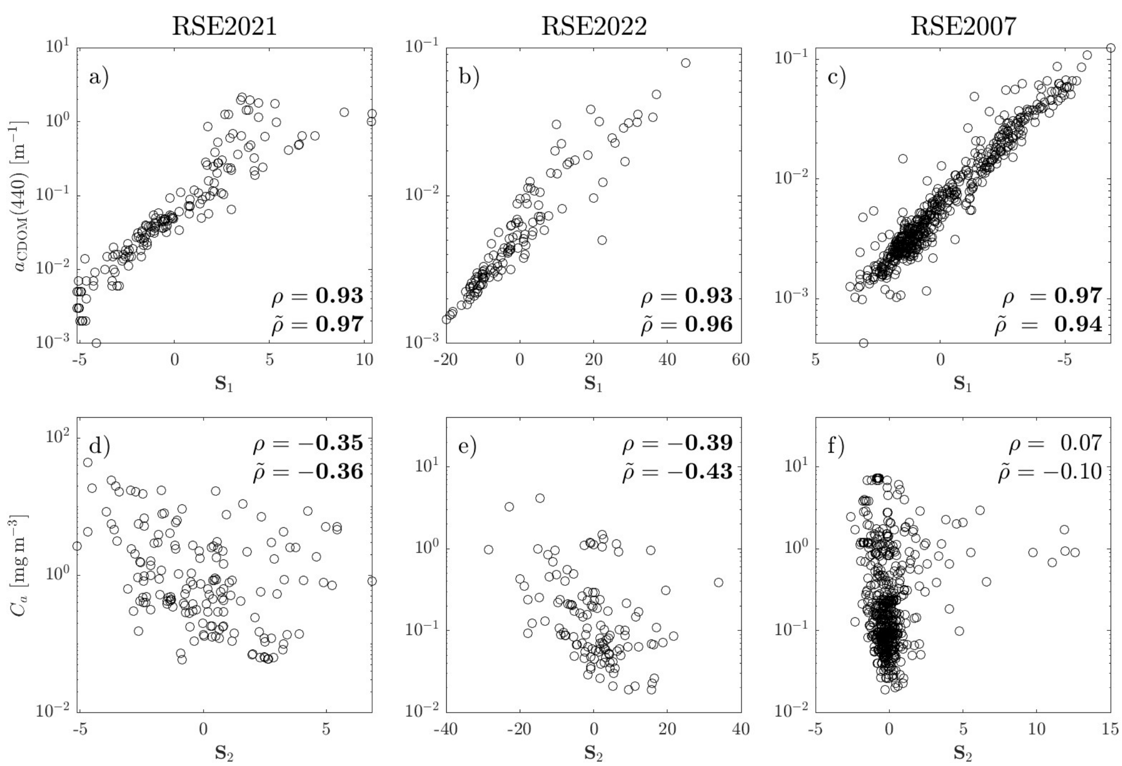

Fig. A2. Relationships between the $\boldsymbol{S}_1$ (top row) and $\boldsymbol{S}_2$ (bottom row) matrix predictors to CDOM absorption (top row) and C_a values (bottom row). Pearson's (ρ) and Spearman's ($\tilde{\rho}$) correlation coefficients are overlaid, with bold type indicating significance at $\mathrm{P} < 0.01$.

The authors add text in the methods section at L269 to clarify that an eigenanalysis characterizes linear patterns of variability, as follows:

> "The eigenanalysis captures linear patterns of variability in the datasets, and is performed, as follows:"

Next, the authors revise L503–505 to incorporate the reviewers point, as follows:

> "For example, considering an idealized case-1 dataset wherein all OACs are accurately derived from C_a, the leading eigenfunction would be anticipated to produce rank correlation coefficients for each OAC. In contrast. . . "

While their analysis provides valuable insights into the primary modes of variability, explicitly discussing these limitations would provide readers with important context for interpreting their findings. This is especially relevant given their conclusion that CDOM, rather than Ca, drives the primary mode of variability in aquatic light fields—a finding that challenges conventional assumptions in ocean color remote sensing.

Authors Response 8: The authors improve the discussions of limitations, as well as clarify elements regarding linearity and algorithm implementation. In Authors Response 7, the authors describe revisions to the text at L269 and L503 to add clarity regarding linearity assumptions of eigenanalyses. The authors also clarify that the eigenfunctions are capturing most of the variance in the dataset, that Spearman's $\tilde{\rho}$ and Pearson's ρ produce similar metrics, and the authors agreed to add the new Fig. A2, which demonstrates linearity between log-transformed $a_{\mathrm{CDOM}}(440)$ and $\boldsymbol{S}_1$. These elements, particularly the relationships shown in Fig. A2, do not support strong nonlinear effects. In addition to the authors' described revisions—including those described at L269 and L503—the authors also add additional discussion of potential limitations within the Conclusion section, described in Authors Response 23.

A last, potentially challenging request: I am going to insist that the authors make the RSE2021 and RSE2022 datasets public, not merely by request. These are too valuable to leave to the chance that the 2 authors become unavailable, etc.

Authors Response 9: The authors acknowledge the reviewer's comment regarding data availability and appreciate the recognition that the RSE2021 and RSE2022 datasets are valuable. Most importantly, the authors fully comply with the data policy of *Biogeosciences*. This policy specifically acknowledges that scenarios arise when "data cannot be deposited publicly." In these circumstances, the policy requires a Data Availability statement to be produced to clearly explains this limitation. As it pertains to the reviewer's comment, the authors are constrained in the full release of the RSE2021 dataset because of a prior data acquisition agreement, and the RSE2022 dataset is already released (and already adequately referenced in the manuscript).

The authors will update the Data Availability statement. To comply with all journal requirements, the authors will also provide a supplementary data file containing the specific data used to generate all figures in the manuscript. The authors believe that this approach is in keeping with both the letter and spirit of the *Biogeosciences* data policy: the authors agree that open data is the ideal, while also acknowledging that there are legitimate situations where complete data sharing is not immediately possible.

Here are some additional, more minor comments for the authors to consider. In order of appearance, not importance:

1. *Include numbers in the Abstract, i.e. be quantitative.*

   Authors Response 10: The authors revise L17–19 of the Abstract, as follows:

   "...Blue and green band-ratio algorithms routinely used for remote sensing of C_a are found to be maximally sensitive to CDOM—rather than C_a—variability based on validation tests of OC algorithm performance (e.g., R^2 of 0.85 versus 0.78), plus partial correlation coefficients relating eigenfunction scalar amplitude functions to field or derived observations."

2. *I encourage the authors to reference Cael+2020 near line 95.*

   Authors Response 11: The authors add a citation for Cael et al. 2020 at L130, as follows:

   "...of the variance—similar information constraint was likewise previously shown for hyperspectral observations of particulate absorption (Cael et al. 2020)."

3. *Line 137: maybe specify that the "optical signatures" are spatial not spectral.*

   Authors Response 12: The authors revise L137, as follows:

   "...airborne investigations leveraged spatially cohesive optical signatures associated with..."

4. *Lines 139-142: The leading components are not always (maybe not even typically) dominated by broadband features. Those are taken out by the mean. One example I know where the first modes are *very* informative are galaxy spectra. Please reword these lines accordingly.*

   Authors Response 13: The authors agree with the reviewer's comment about the first modes being informative—the implication of the first mode is fundamental to the results herein. This statement instead describes a potential pitfall in quantifying information content based on eigenanalyses: Processes or constituents that modify spectra across an expansive wavelength range mathematically receive more weight in an eigenanalysis than those that modify only a narrow spectral region. Therefore, the results of an eigenanalysis may sometimes not adequately reflect information associated with processes that modify a narrow spectral region. The authors clarify this by revising L139–141, as follows:

   > "Quantifying information content using eigenanalyses can likewise be challenging: dimensionality bias can produce an incomplete perspective of information content by increasing the variance captured by broadband features relative to that of narrow features. The latter—when not spectrally diluted—often provide informative and exploitable information (Houskeeper et al. 2020b)."

5. *Somewhere in the last paragraph of the Introduction, I encourage the authors to cite the recent papers by Z. Erickson (2020 and 2023).*

   Authors Response 14: The authors revise L141–143, as follows:

   > "Mixture density networks (MDNs) and inverse models that incorporate prior knowledge (i.e., leveraging a Bayesian framework) improve the management of degeneracy in radiative transfer, and are forthcoming for PACE science objectives (O'Shea et al. 2021; Erickson et al. 2020,2023)."

6. *Somewhere, consider citing Siegel+2013 as a previous reference showing/asserting that CDOM dominates absorption at bluer wavelengths.*

   Authors Response 15: The authors previously cited Jerlov (1968) on L320–321. Following the reviewer's preference, the authors add Siegel et al. (2013):

   > "Conversely, spectral darkening of shorter wavelengths with minimal spectral features is most consistent with CDOM absorption (Jerlov 1968; Siegel et al. 2013)."

7. *Line 313: Please cite a reference supporting the assertion that "scattering processes confer less spectral dependencies."*

Authors Response 16: The authors add a citation for Kirk (2011), which provides a useful review on this topic, and also add text to reference absorption band effects for completeness, as follows:

> "The spectral shapes of the eigenfunctions are primarily considered as a function of absorption processes, which generally—notwithstanding absorption band effects (Zaneveld and Kitchen 1995)—confer stronger spectral dependencies than scattering processes (Kirk 2011)."

8. *Line 373: I have to admit I am not familiar with the term "R2 statistics."*

Authors Response 17: The authors replace "R^2 statistics" with "R^2" following the reviewer's preference.

9. *Line 436: I struggle to parse this paragraph. Found myself mainly confused reading it. Maybe provide additional context?*

Authors Response 18: The discussion is related, in part, to the reviewer's earlier questions regarding nonlinearities in aquatic optics. The authors revise the paragraph to improve clarity and reduce length plus complexity, as follows:

> Bio-optical formulations to derive optical properties as a function of C_a do not require primacy of C_a. Rather, algorithms parameterize evolution in optical properties—notwithstanding observational challenges—based on empirical OAC relationships (Morel and Prieur 1977; Morel 2009). Nonetheless, variability in OAC relationships exists for *in situ* water bodies (Hansell and Orellana 2021). Empirical approaches such as the OC family of algorithms must mitigate observational artifacts (Uitz et al. 2006; Kudela et al. 2019, 2024), plus regional variability and nonlinearity in OAC relationships (Morel 2009). The latter manifests with the need to regionally tune VIS algorithms for specific waters. For example, tunings for arctic waters account for higher $a_{\mathrm{CDOM}}(440)$ relative to C_a content (Matsuoka et al. 2013; Lewis and Arrigo 2020), and tunings for antarctic waters account for lower $a_{\mathrm{CDOM}}(440)$ relative to C_a (Dierssen and Smith 2000). The latter is also in keeping with highly nonlinear formulations of OC algorithms, e.g., the number of power terms used in the polynomial model to fit C_a to ratios of R_{rs} is routinely four (Morel 2009; O'Reilly and Werdell 2019). Linearity and loglinearity of CDOM algorithms increases with increasing spectral separation of wavelengths (Hooker et al. 2020, 2021a; Houskeeper et al. 2021). The results herein suggest that differences in linearity correspond, in part, to differences in the separability of signals associated with spectral range.

10. *Line 447: "are stable" –> "are [un]stable" ?*

Authors Response 19: The original usage, i.e., stable, was correct, but the authors revise this paragraph to improve clarity and reduce length, as described in Authors Response 18.

11. *Line 460: I was not persuaded that item c) was actual, independent evidence*

Authors Response 20: The authors revise this text to help clarify their meaning, i.e., that their findings are supported by both the variance captured by the leading and secondary eigenfunctions, as well as the correlations observed between the $\boldsymbol{S}$ matrixes and the biochemical parameters. The latter is also further clarified by Fig. A2. The authors reorganize L455–465, as follows:

> "The similarities favor primacy of $a_{\text{CDOM}}(440)$—rather than C_a—as the predominant driver of optical variability for waters, including those of the open ocean, summarized briefly, as follows: a) the leading eigenvector from each dataset—capturing approximately 60% of the variance—indicates opposing anomalies for longer versus shorter wavelengths with minimal amplitude in the blue-green transition domain. The secondary eigenvector from each dataset—capturing approximately 32% of the variance—indicates internal VIS spectral dependencies characteristic of C_a absorption, including a maximum near the blue-green transition; b) the $\boldsymbol{S}_1$ term representing the stretching and compressing necessary to best represent the data using the leading eigenfunction is always more strongly associated with variability in $a_{\text{CDOM}}(440)$ than C_a values. The $\boldsymbol{S}_2$ term more strongly associates with field observations of C_a than $a_{\text{CDOM}}(440)$ for two of the three datasets..."

12. *Lines 489: I encourage authors to include equations describing the processes written about here.*

Authors Response 21: The reviewer has requested that the authors include an equation regarding L489, which describes the negative buoyancy of particles—which is parameterized following Stokes law (1851). While the authors are generally supportive of including equations, the authors perceive sinking rate parameterizations as only indirectly relevant to the manuscripts findings. The authors will therefore add clarity regarding the reviewer's comment by adding text, plus a citation regarding the following line which the reviewer also may have been intending. The authors perceive that this revision helps clarify the material without adding unnecessary complexity. The authors revise L489–490, as follows:

> "Spatial differences occur, perhaps, due to negative buoyancy of particles—e.g., sinking velocity increases proportionally with density differences and the squared particle radius (Bach et al., 2012)—driving particulate organic distributions away from the surface where remote sensing signals are weighted (e.g., Morel and Berthon 1989)."

13. *Line 560: Consider citing Prochaska & Frouin (2025) here.*

Authors Response 22: The authors add Prochaska and Frouin (2025) at L560. Based on additional revisions described in Authors Response 30, the full revision at L569 is as follows:

> "Accurate retrieval of $a_{\mathrm{CDOM}}(440)$ is, therefore, prerequisite to—not separate from—accurate retrieval of phytoplankton properties, in keeping with the trajectory of research into simultaneous inherent optical property (IOP) inversions (e.g., Maritorena et al. 2022; Lee et al. 2002; Werdell et al. 2013), machine learning approaches (O'Shea et al. 2021), and degeneracy (Prochaska and Frouin 2025)."

14. *The conclusions are largely summary + self-promoting. If that is the standard for this Journal, no problem.*

Authors Response 23: While the *Biogeosciences* submission guidelines do not provide any specialized requirements relating to the composition of the Conclusion section (https://www.biogeosciences.net/submission.html), the authors appreciate this feedback on the Conclusion text. The authors revise the Conclusions section, as follows:

> "~~Spectral observations of aquatic environments produce leading eigenfunctions of AOPs more strongly correlated to variability in CDOM absorption than C_a.~~ Greater independence of OACs and the elevated importance of CDOM variability in governing aquatic light variability are consistent with advancing knowledge of microbial loop dynamics and an increasing diversity of trophic pathways represented therein (Azam 1998). The consistency of results using three independent datasets strengthens support for ~~and are based on consistent results for the eigenanalyses—including the spectral shapes of the eigenfunctions and the partial correlation coefficients relating the eigenfunctions to biogeochemical variables—plus performance metrics of OC algorithms. The eigenanalyses indicate~~ accurate and independent estimation of CDOM as prerequisite to retrieval of C_a and other phytoplankton parameters. However, not every bio-optical dataset, quality control protocol is assessed, not all applicable OACs are present in the datasets, and the eigen analyses capture linear—but not nonlinear—patterns of variability. ~~and satellite OC algorithms are found herein to produce values more highly correlated with CDOM than C_a.~~ Confounding signals identified for CDOM and C_a are consistent with early investigations into the drivers of color variability (Yentsch 1960), as well as subsequent work assessing vulnerabilities in band-ratio algorithms for characterizing C_a (Dierssen 2010; Sauer et al. 2012). Spectrally expansive data products have been shown to improve retrieval of $a_{\mathrm{CDOM}}(440)$ independent of C_a (Sathyendranath

et al. 1987; Hooker et al. 2020; Houskeeper et al. 2021), and comparisons herein of eigenanalyses using ~~the INV21 and VIS21~~ complete spectra versus spectral subsets further support potential opportunities associated with spectral range expansions. Spectrally expansive data products have been demonstrated *in situ* spanning the UV to shortwave infrared (SWIR) wavelength domain, with the latter formerly ascribed as null ~~in the ocean color community of practice~~ (Houskeeper and Hooker 2023). The recently launched OCI sensor of the PACE mission provides hardware capabilities to support expansive spectral range observing of the global ocean surface. The findings herein support opportunities associated with leveraging the spectrally expansive capabilities of OCI, although further advances in image processing, atmospheric correction, algorithm design, and ~~applicability of~~ *in situ* datasets would be necessary."

The authors thank Reviewer 1 for their comments and suggestions, which helped the authors to improve the manuscript.

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Authors Response to Reviewer 2 Comments for Manuscript egusphere-2024-4163: *The primacy of dissolved organic matter to aquatic light variability*

9 May 2025

The authors thanks Reviewer 2 for their valuable comments. The authors respond to all comments below and document resulting modifications to the manuscript, as appropriate. Reviewer 2's comments are shown in *slanted* typeface. The Authors Responses are shown in plain typeface. The numbering of the Authors Responses continues from the numbering of the Authors Responses to Reviewer 1 to minimize ambiguity when referencing across response documents. Revised or added text is indicated in red. All line numbers are indicated with a capital "L" and refer to the line numbers in the original submitted work. Citations within this response document correspond to the References section at the end of this document.

Comments from Reviewer 2:

The manuscript proposes a change in paradigm in ocean color remote sensing, providing evidence that CDOM absorption—rather than Ca—primarily drives water-leaving light variability. They additionally make a strong case for exploiting information in the INV range of the spectra, clearly highlighting current limitations in both in situ and satellite datasets. The work has potentially great scientific implications, as it could change the way that aquatic light variability is thought, and ocean color algorithms are designed. However, I believe that the authors should address some comments detailed below to make their point stronger.

Authors Response 24: The authors thank the reviewer for their positive and constructive comments.

The authors acknowledge the important role of different OACs in the variability of aquatic light, with the purpose of ultimately demonstrating the primacy of CDOM over Ca. OACs in water are typically grouped in three different categories: CDOM, phytoplankton and non-algal particles (NAP) that can covary or not. However, the work does not assess the potential contribution of non-algal particles (NAP) to light variability (apart from briefly mentioning inorganic particles in lines 410-412). How relevant are NAPs in the study's datasets? Can their contribution be reasonably neglected? If so, this needs to be clearly justified. How does this omission in the datasets limit the findings of the work? How about the extrapolation of the findings to waters where NAPs contribution may be more relevant.

Authors Response 25: The authors agree with the reviewer regarding the importance of NAPs to aquatic light variability. Correlation coefficients relating the principal component time series to NAP variability were not presented because coincident observations of NAPs were not available. The challenge stems, in part, from the paradigm noted by the reviewer in their initial comment: Chlorophyll a (C_a) is generally considered the primary variable in ocean color. As a result, C_a is often the primary—and sometimes only—biogeochemical field measurement obtained to accompany observations of apparent optical properties (AOPs). The RSE2021 dataset was able to add routine measurements of $a_{\mathrm{CDOM}}(440)$, which, in part, made this study into the primacy of $a_{\mathrm{CDOM}}(440)$ possible.

However, despite the challenging deficiency in observations of NAPs for many applicable datasets, the RSE2021 dataset presented herein does capture substantial variability in NAP based on water bodies sampled. For example, many riverine systems frequently contain high concentrations of suspended sediments, and examples of sediment-rich rivers—namely the Colorado, Napa, and Columbia rivers—are represented in the RSE2021 eigenanalysis. Similarly, an expansive range in NAP is represented by lacustrine waters sampled spanning Crater Lake (OR) to Pinto Lake (CA), plus the sampling or estuaries such as Elkhorn Slough (CA) and San Francisco Bay (CA). This is not true for the RSE2022 or RSE2007 datasets, which did not include inland waters, and so the similarity in variance captured by the leading eigenfunction for all datasets (within $\pm 1\%$) suggests that NAPs are not strongly modifying the leading eigenfunction of RSE2021. This scenario is similar to the discussion of detrital absorption in Authors Response 4.

For a previous publication, the authors derived estimates of the coefficient for particulate backscattering at 443 nm, $b_{\mathrm{bp}}(443)$, based on an inversion scheme applicable to case-1 and case-2 waters (Matsuoka et al. 2013) and with updates for coastal waters (Hooker et al. 2021a). The estimation indicates an expansive range in $b_{\mathrm{bp}}(443)$ spanning 0.001 to $0.329\,\mathrm{m}^{-1}$. Combined with the representation of riverine, lacustrine, and estuarine water bodies wherein inorganic particle concentrations were highly variable, the $b_{\mathrm{bp}}(443)$ range indicates that the RSE2021 eigenanalysis is anticipated to capture a non-negligible amount of *in situ* variability associated with NAPs. The authors show the dataset quartile characteristic for the synthetic $b_{\mathrm{bp}}(443)$ coefficients in Table A1 (also discussed in Authors Response 29) to clarify elements of NAP representation by RSE2021. The authors do not test the $\boldsymbol{S}$ matrix values against the synthetic $b_{\mathrm{bp}}(443)$, because this could contribute to misinterpretation based on presently uncharacterized dynamics of the $b_{\mathrm{bp}}(443)$ algorithm performance, which is outside the scope of the submitted manuscript.

Next, the authors note that the leading eigenfunction of the RSE2021 dataset explained 0.60 of the variance in the dataset. The leading eigenfunction produced a spectral shape similar to CDOM absorption and also indicated very high linear correlation to $a_{\mathrm{CDOM}}(440)$ with $r = 0.92$ (the somewhat lower value of 0.80 shown in Fig. 1 is a partial correlation value that includes accounting for effects of C_a, discussed in Authors Response 39), or an r^2 of 0.85. This suggests (approximately) that $a_{\mathrm{CDOM}}(440)$ captures on the order of 0.85 of the 0.60 captured by $\boldsymbol{\psi}_1$, which amounts to 0.51. Even if all other variance in the dataset was driven by a single other OAC (e.g., C_a, NAP, but also a_{phy} referencing Authors Response 26), the OAC could not achieve primacy because only 0.49 of the total variance remains. For the INV domain, the results are much stronger and suggest $a_{\mathrm{CDOM}}(440)$ captures greater than 0.70 of the variance. The results of these comparisons, therefore, do not suggest primacy of NAPs for the datasets tested herein.

The results of the datasets herein correspond to large-scale (e.g., global) dynamics. Targeted subsets of these datasets would *not* necessarily show similar importance of $a_{\mathrm{CDOM}}(440)$. For example, lacustrine datasets with a wide range in C_a—e.g., combining Crater Lake, (CA) and Clear Lake (CA)—might be anticipated to produce spectral variability most associated with C_a. Similarly, an onshore to offshore transect from the mouth of the Rio de la Plata—wherein very high suspended sediments injected into the coastal ocean by river discharge are mixed and diluted with oceanic water—might be anticipated to produce spectral variability most associated with changes in suspended sediment concentrations. The authors clarify that the results of the large-scale analyses do not apply to individual or regional scenarios by adding discussion after L515, as follows:

> "The findings presented herein correspond to datasets spanning globally representative or broad oceanic waters, and do not rank the importance of drivers in any specific region. For example, regional scenarios wherein high variability of non-algal particles (NAPs) is associated with riverine flux or resuspension would not be anticipated to reflect the findings herein supporting $a_{\mathrm{CDOM}}(440)$ primacy."

The authors also agree with the reviewer that not having field observations of b_{bp} or NAP (or detrital absorption, as described in Authors Response 7) is an important limitation to address. The authors clarify that the findings indicate high importance of CDOM absorption—despite the effects of C_a but also NAP and other OACs—but that adding field sampling of other OACs would help strengthen the analysis and provide more opportunities to explore additional relationships. The authors add discussion at L515, as follows:

> "The findings demonstrate high variance captured by the leading eigenfunction and the eigenfunction's strong association with $a_{\mathrm{CDOM}}(440)$ variability, but the findings would be strengthened by adding field sampling for additional biochemical or bio-optical parameters. For example, RSE2021 demonstrates the importance of combining spectrally expansive radiometry and observations of C_a with observations of $a_{\mathrm{CDOM}}(440)$. Also adding observations of non-algal particles (NAPs) and detrital absorption would help to further improve clarity on the eigenfunction interpretations, and, perhaps, contribute to a better understanding of the subsequent modes."

CDOM absorption coefficient (aCDOM) is an optical property itself, more directly related to Lw than Ca. Therefore, one could argue that it would be fairer to use phytoplankton absorption (aphy) rather than Ca in this study. They additionally have another important difference: while the spectral shape of CDOM absorption is smooth and can be roughly defined by two quantities (aCDOM at a reference wavelength, e.g., 440 nm, and an exponential decay exponent), aphy can present much more spectral variability in natural waters, not being as easily parameterized. Can these differences give an "advantage" to CDOM in the analyses presented in the manuscript, particularly when computing linear correlation coefficients with the eigenfunctions? Please include any pertinent discussion about this.

Authors Response 26: Similar to detrital absorption (Authors Response 4) and NAP (Authors Response 25), the authors are constrained by the sampling activities of globally representative radiometric datasets and their corresponding field observations—but the analyses nonetheless are informative regarding other OACs. For example, the likelihood of a scenario wherein variability in C_a to a_{phy} could alter the findings presented herein is challenged by the strength of the results concerning $a_{\mathrm{CDOM}}(440)$—including the variance calculations discussed in Authors Response 25. Briefly, the results presented herein support very high correlation of the leading eigenfunction to log-transformed $a_{\mathrm{CDOM}}(440)$, i.e., greater than 0.9 for the RSE2021, RSE2022, and RSE2007 datasets. The relationships to $a_{\mathrm{CDOM}}(440)$ are also highly linear, shown in Fig. A2 (introduced in Authors Response 7), which also presents Pearson's correlation coefficient (ρ) and Spearman's rank correlation coefficient (herein $\tilde{\rho}$) side-by-side for comparison:

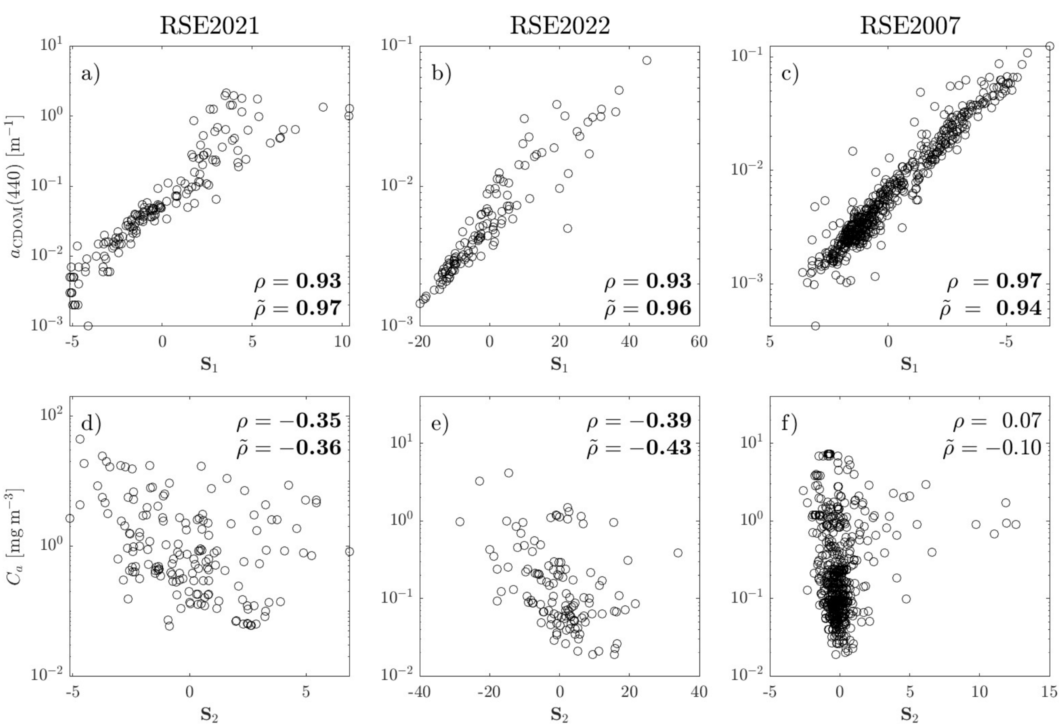

Fig. A2. Relationships between the $\boldsymbol{S}_1$ (top row) and $\boldsymbol{S}_2$ (bottom row) matrix predictors to CDOM absorption (top row) and C_a values (bottom row). Pearson's (ρ) and Spearman's

($\tilde{\rho}$) correlation coefficients are overlaid, with bold type indicating significance at P < 0.01.

The partial correlation coefficients presented in Fig. 1 for $a_{\mathrm{CDOM}}(440)$ and C_a as they relate to the leading eigenfunction are also quite disimilar. For example, RSE2021 indicates that correlation of $a_{\mathrm{CDOM}}(440)$ to the leading eigenfunction (and accounting for covariance with C_a) is 0.80. The opposite comparison—correlation of C_a to the leading eigenfunction and accounting for covariance with $a_{\mathrm{CDOM}}(440)$—is 0.11. The magnitude of these differences (0.80 versus 0.11) does not support the results being dependent on variability in C_a to a_{phy}, which are generally highly correlated. For example, as described in Roesler and Barnard (2013):

> "The line height absorption is shown to be significantly related to the extracted chlorophyll concentration over a large range of natural optical regimes and diverse phytoplankton cultures."

The spectral shape of a_{phy} is also routinely derived from C_a (Morel 2009), i.e., consistent with the focus herein on assessing the validity of C_a primacy. The authors clarify potential sources of variability in the relationship between C_a and phytoplankton absorption by adding discussion to L453, as follows:

> "Phytoplankton absorption—rather than C_a—was not tested due to the limitations of the datasets. Although phytoplankton absorption is generally considered to correspond to C_a, processes such as pigment packaging can add variability relevant to the correlations presented herein (Bricaud et al. 2004)."

Following the previous comments, why did the authors decide to use only Pearson correlation? I suggest they consider including (additionally) a non-linear correlation coefficient (e.g., Spearman's rank correlation). This could enrich the results and discussion.

Authors Response 27: The authors add Spearman's rank correlation in Fig. A2, which they also describe in Authors Response 7 of their responses to Referee 1. The authors find that the results from Spearman's rank correlation are extremely similar to those using Pearson's rank correlation. The authors show the Spearman's rank correlation values in Fig. A2, which also shows that the relationships between the $\boldsymbol{S}_1$ matrix and log-transformed $a_{\mathrm{CDOM}}(440)$ are highly linear. The authors thank the reviewer for the suggestion to also add Spearman's rank correlation.

I think the work could greatly benefit from exploiting the datasets a bit more, complementing the results of the principal components analysis. For example:

1. *For completeness and better contextualization, I suggest including a figure with the measured spectra when describing each dataset, so the reader can have a quick visualization of the spectral variability represented in the work.*

   Authors Response 28: Fig. A1, as described in Authors Response 6, presents the mean spectra from each dataset, plus the shapes of the changes associated with each eigenfunction. The authors believe that these examples are more informative given the high quantity and overlap of the spectra, combined with the eigenfunctions in Fig. A1 representing 97% of the variance in the datasets.

2. *It would also be beneficial to report the correlation coefficient between aCDOM and Ca in the considered datasets, as well as a table with the median, quartiles and ranges of aCDOM and Ca measurements. Could it be the case that aCDOM can "explain" more variance because it already had greater variability in the datasets, while Ca varied in a more limited range (maybe it is necessary to consider some relation between aphy and Ca to do this comparison)?*

   Authors Response 29: The reviewer makes multiple good points, and the authors address each element, as follows:

   - *Report the correlation coefficient between aCDOM and Ca in the considered datasets:*

     The authors add text stating the correlation coefficients for $a_{\mathrm{CDOM}}(440)$ and C_a to L287:

     > "...captured by a remote sensing algorithm. Pearson's correlation coefficients comparing C_a and $a_{\mathrm{CDOM}}(440)$—measured or derived algorithmically—are 0.812, 0.912, and 0.909 for the RSE2021, RSE2022, and RSE2007 datasets, respectively."

   - *[Add] a table with the median, quartiles and ranges of aCDOM and Ca measurements:*

     Table A1 at the end of this Authors Response shows the requested information—plus synthetic $b_{\mathrm{bp}}(443)$ to also expand on Authors Response 25.

   - *Could it be the case that $a_{\mathrm{CDOM}}(440)$ can "explain" more variance because it already had greater variability in the datasets, while C_a varied in a more limited range?*

     The authors investigate this scenario and confirm it is not supported based on comparison of dynamic ranges expressed in the datasets. Briefly, $a_{\mathrm{CDOM}}(440)$ confers greater dynamic range than C_a in the RSE2007. C_a confers greater dynamic range than $a_{\mathrm{CDOM}}(440)$ in

RSE2022. $a_{\mathrm{CDOM}}(440)$ and C_a confer the same number of decades of dynamic range in RSE2021. Although scenarios wherein variability in $a_{\mathrm{CDOM}}(440)$ is greater, less than, or comparable to that of C_a arise, the results indicating primacy of $a_{\mathrm{CDOM}}(440)$ are consistent across datasets. The authors add discussion at 467 to discuss the dynamic range expressed in the biochemical quantities for the datasets, as follows:

> "The datasets assess herein represent $a_{\mathrm{CDOM}}(440)$ spanning greater, lesser, or comparable dynamic range compared to C_a, indicating that the result of $a_{\mathrm{CDOM}}(440)$ primacy is not associated with differences in the dataset ranges of the biochemical constituents."

Table. A1. The quartile summary of biogeochemical quantities from the RSE2021, RSE2022, and RSE2007 dataset field observations, plus estimated values for $b_{\mathrm{bp}}(443)$ derived following Matsuoka et al. (2013) and Hooker et al. (2021a). Out-of-bound values are indicated as limit of detection (LOD).

Dataset	Parameter	Min	Lower Quartile	Median	Upper Quartile	Max
$a_{\mathrm{CDOM}}(440)$ $[\mathrm{m}^{-1}]$	RSE2021	0.0010	0.0175	0.4550	0.2185	2.1460
	RSE2022	0.0015	0.0028	0.0044	0.0088	0.0795
	RSE2007	0.0004	0.0027	0.0040	0.0124	0.1242
C_a $[\mathrm{mg\,m^{-3}}]$	RSE2021	0.0590	0.2925	0.7440	2.690	44.1960
	RSE2022	0.0190	0.0580	0.1015	0.2520	4.1510
	RSE2007	0.0190	0.0780	0.1450	0.4815	7.3180
$b_{\mathrm{bp}}(443)$ $[\mathrm{m}^{-1}]$	RSE2021	LOD	0.0010	0.0050	0.0290	0.3290

3. *Finally, I suggest the authors include an example of improved Ca retrieval after determining aCDOM first. I know this is a non-trivial and challenging request, but I think it would be a very convincing proof that the change of paradigm is necessary.*

Authors Response 30: The authors acknowledge the reviewer's point, but respectfully do not perceive that adding an example of C_a retrieval would improve the manuscript. The authors summarize four main reasons for their perspective, as follows:

First, improving phytoplankton biomass estimation (e.g., C_a) via simultaneous or prior estimation of dissolved organic absorption is very well documented in the literature. Briefly, the topic supports the development of so-called semi- and quasi-analytical algorithms—including the Generalized Inherent Optical Property (GIOP), Garver Siegel Maritorena (GSM), and Quasi-Analytical Approach (QAA) algorithms (e.g., Maritorena et al. 2022; Lee et al. 2002; Werdell et al. 2013)—and is inherent in machine-learning approaches (e.g., O'Shea et al. 2023). In these and many other instances, advances in quantifying phytoplankton biomass is shown via corresponding retrieval of dissolved organic (and other) optical properties.

The authors will improve clarity of the historical context, by modifying L560–561, as follows:

> "Accurate retrieval of $a_{\mathrm{CDOM}}(440)$ is, therefore, prerequisite to—not separate from—accurate retrieval of phytoplankton properties, in keeping with the trajectory of research into simultaneous inherent optical property (IOP) inversions (e.g., Maritorena et al. 2022; Lee et al. 2002; Werdell et al. 2013), machine learning approaches (O'Shea et al. 2021), and degeneracy (Prochaska and Frouin 2025)."

Second, demonstrating that C_a retrieval is improved by first determining $a_{\mathrm{CDOM}}(440)$ is documented by Fig. 2. In this figure, all three datasets indicate higher R^2 values for C_a estimation using an $a_{\mathrm{CDOM}}(440)$ algorithm (panels d–f) compared to that derived using the OC algorithm (panels a–c). In other words, Fig. 2 proves that estimation of C_a improves when $a_{\mathrm{CDOM}}(440)$ is derived first, because Fig. 2 shows that a loglinear fit of algorithmic $a_{\mathrm{CDOM}}(440)$ improves C_a estimation. The manuscript states on L384–386:

> "Although the differences observed are slight for RSE2007 (indicating the dataset adheres well to case-1 waters), all datasets nonetheless produce stronger R^2 statistics when comparing the OC algorithm values to $a_{\mathrm{CDOM}}(440)$ versus C_a."

Third, the suggestion would unnecessarily expand the scope of the submitted manuscript, which already approaches 20 pages without including figures or other revisions described herein. Responsibly producing a C_a algorithm would also require much more analysis to ensure that the observations being fit—as well as the fitting procedure—produce C_a estimations that are representative of natural waters. The C_a algorithm would also require addition of substantial new text to describe the quantification of uncertainties and define the limitations for the new C_a approach.

Comments from another reviewer also provide an example as to why the authors do not anticipate that adding a new approach for estimation of C_a would be beneficial: algorithms produced to investigate a topic or provide an example can also reduce clarity of a manuscript or cause confusion later. For example, a notebook analysis discussed in Authors Response 3 invokes algorithms (e.g., the blue and green dots from the link in Authors Response 3) that were previously produced for comparison purposes to investigate whether dissimilar datasets—corresponding to significant differences in data quality and bias—produce similar degradations in algorithmic performance when the spectral range of the algorithmic relationship is decreased.

Fourth, the authors perceive that adding a new method for estimating C_a would decrease the clarity of the manuscript by redirecting the focus towards C_a estimation and ocean color algorithm development.

Other minor and more specific comments are:

- *The references throughout the manuscript to "end-member analysis (EMA)" are somewhat confusing. At first I thought that it was a stablished methodology (the term is actually used in other disciplines), but then I realized that it is unrelated to the methodologies used in other disciplines, and it rather seems to refer to a type of algorithm developed by the authors in previous works, referring to the use of wavebands in the extremes of the spectra to estimate CDOM absorption. I think this should be clearly stated in the manuscript to avoid any confusion.*

  Authors Response 31: The authors clarify on this point by defining end-member analysis at its first usage. The authors revise L106–107 (also described in Authors Response 2), as follows:

  > "...based on using ratios of the most spectrally separated optical data products (Hooker et al. 2013), especially those from the UV and NIR spectral domain, an approach hereafter termed end-member analysis (EMA) following Hooker et al. (2020). Conservative waters..."

- *Lines 19-20: "Spectral subset eigen analyses indicate expansive spectral range observing improves the independence in retrieving CDOM absorption and Ca." I cannot understand this sentence, please rephrase it.*

  Authors Response 32: The authors revise L19–L20, as follows:

  > "Eigenanalyses applied to spectral subsets of the data indicate expansive spectral range observing improves the independence in retrieving CDOM absorption and C_a."

- *Lines 58-84: Although I find the information summarized in these paragraphs very interesting, I do not think that the level of details included here is necessary, particularly because it does not flow with the reading of the previous and following paragraphs. I would recommend shortening this part and reducing the number of citations to those only necessary to support the current work.*

Authors Response 33: The authors perceive this material as necessary to understand the differences in bias between the *in situ* datasets leveraged herein. To improve flow based on the reviewer's comment, the authors shorten and re-organize this material so that the discussion occurs nearer to existing methodological discussion of the *in situ* datasets. The authors remove L71–84 and add a portion of this text at L189, as follows:

> "...approximately the length of the downward-pointing radiance radiometer (Hooker et al. 2020). Improvements in sampling rates support management of high-frequency, non-Gaussian variability in flux observed by an above- or in-water instrument (due to glint and wave focusing, respectively), thereby expanding the spectral range of optical data products to preserve INV information and retaining information associated with spectral signal amplitudes or brightness (Houskeeper et al. 2023; 2024).
>
> SOTA advances in hyperspectral instrumentation include hybridspectral sensing configurations (Hooker et al. 2022), wherein microradiometer and spectrograph observations are obtained in concert, with the multispectral microradiometer providing necessary quality control for the hyperspectral spectrograph. The quality control is desirable, in part, because COTS spectrographs suffer from slower integration times, narrower dynamic range, and a degraded signal-to-noise ratio (SNR) relative to COTS microradiometers (Houskeeper et al. 2024; Kudela et al. 2019; 2024). In addition, a radiance control arm positions the $L_u(z,\lambda)$ aperture near the water surface and approximately aligned with the upward-pointing irradiance radiometer (Hooker et al. 2018a). Improvements in the number of spectrograph pixels to as high as 2,048..."

This also requires minor revisions to L120 to preserve presentation of acronyms, as follows:

> "...preclude most non-visible—or invisible (INV)—data products..."

As well as to and L101:

> "...spectral range, resolution, and signal-to-noise ratio (SNR) of legacy ocean color datasets..."

- *Line 84: The reference to Ruddick et al. (2023) is missing.*

Authors Response 34: The authors thank the reviewer for catching the missing reference. The Ruddick et al. 2023 citation is removed in Authors Response 33.

- *Line 104, 154: I am not familiar with the expression "spectrally expansive", if this is well-known terminology, please disregard this comment, otherwise, I suggest to briefly define what the authors mean by this.*

  Authors Response 35: The authors add a sentence defining spectrally expansive following its first usage on L104, as follows:

  > "Spectral *expansivity* herein refers to the spectral range of (compliant) data products, with the most spectrally expansive observations corresponding to those representing the greatest spectral range."

- *Lines 151, 199, 204, 210, 221, etc. What are contemporaneous measurements? Do you mean simultaneous?*

  Authors Response 36: The authors revise the text to define contemporaneous—following the Merriam-Webster dictionary—at its first usage on L63, as follows:

  > "...This era of development also included contemporaneous—i.e., occurring during the same time—advances in...."

- *Line 268: "the square root transformation improves normality" Why? Is there a reference to support this assertion?*

  Authors Response 37: Transforming a dataset using, e.g., the natural logarithm can be helpful for improving normality so that the assumptions of some parametric statistical tests are approximately satisfied. Normality may be assessed, e.g., by visually inspecting histograms of the data products, as well as using metrics such as the Shapiro-Wilk test statistic, W, wherein values closer to 1 indicate normality.

  In their study, the authors tested various transformations of the different datasets using W and found that no one transformation type was optimal across all wavelength domains. Overall, the authors found that W was maximal in the longer wavelength domain (> 500nm) if logarithmic transformation were applied, and maximal in the shorter wavelength domain (< 500nm) if root transformations were applied. The authors applied a square-root transformation because most absorption variability in aquatic optics is associated with the blue (< 500nm) domain (e.g., Chase et al. 2013). In addition, the authors performed sensitivity testing to test whether the results were insensitive to the transformation type. Briefly, natural-log transformation, square-root transformation, and no transformation all produced eigenfunctions with the same approximate spectral shapes.

  The authors revise L268 to clarify this topic, as follows:

> "…observations of the square root of $\left[L_W(\lambda)\right]_{\mathrm{N}}$, hereafter $[L_W(\lambda)]_{\mathrm{N}}^{0.5}$, because the square-root transformation was found to improve normality in the blue spectral domain based on the Shapiro-Wilk test statistic, W. Sensitivity testing was performed by reproducing the eigenanalyses using natural-log transformation, as well as no transformation, to assess whether the spectral shapes of the eigenfunctions were approximately insensitive to the transformation treatment."

- *Lines 270-276: I must admit that I am not very familiar with PCA applied to spectral datasets, and it would have greatly helped if the authors included matrices dimensions in equations (3) and (4).*

  Authors Response 38: The authors revise the text to add dimension information based on the reviewer's comment. First, the authors revise L271, as follows:

  > "…in which $\boldsymbol{C}$ is the covariance matrix of the $[L_W(\lambda)]_{\mathrm{N}}^{0.5}$ values for each dataset, with square dimensions, each corresponding to the number of wavelengths in each dataset. The $\boldsymbol{\psi}$ value denotes…"

  Next, the authors revise L278, as follows:

  > "…(where i is the eigenfunction index). The length of each $\boldsymbol{S}_i$ column is the number of observations in the underlying dataset."

- *Line 283-284: "after adjusting for covariance with the biogeochemical quantity y." How was this done? Please describe or add a reference.*

  Authors Response 39: Adjusting the correlation coefficient for covariance with another quantity is a statistical technique termed the partial correlation coefficient. The authors add a reference, plus re-organize L281–284 to add clarity, as follows:

  > "Because biogeochemical parameters covary, e.g., C_a and $a_{\mathrm{CDOM}}(440)$ are strongly correlated (Morel and Prieur 1977), partial correlation coefficients (Fisher 1924) are derived using notation wherein $\rho_{i,x|y}$ indicates correlation of $\boldsymbol{S}_i$ with biogeochemical quantity x after adjusting for covariance with the biogeochemical quantity y."

- *Lines 335: "or fluorescence properties" instead of "of fluorescence properties"?*

Authors Response 40: The authors thank the reviewer for catching this typo. The authors revise the text on L335, as follows:

> "...the spectral domains of C_a absorption or fluorescence properties."

- *Lines 438-440: I do not understand the sentence that begins with: "The variability may, perhaps, correspond in part to..." I do not follow the connection with the previous sentence. Please rephrase it.*

Authors Response 41: The authors agree that this sentence should be revised to improve clarity, and revisions to the sentence (and paragraph in which this sentence occurs) are described in Authors Response 18. The revision is, as follows:

> "Bio-optical formulations to derive optical properties as a function of C_a do not require primacy of C_a. Rather, algorithms parameterize evolution in optical properties—notwithstanding observational challenges—based on empirical OAC relationships (Morel and Prieur 1977; Morel 2009). Nonetheless, variability in OAC relationships exists for *in situ* water bodies (Hansell and Orellana 2021). Empirical approaches such as the OC family of algorithms must mitigate observational artifacts (Uitz et al. 2006; Kudela et al. 2019, 2024), plus regional variability and nonlinearity in OAC relationships (Morel 2009). The latter manifests with the need to regionally tune VIS algorithms for specific waters. For example, tunings for arctic waters account for higher $a_{\mathrm{CDOM}}(440)$ relative to C_a content (Matsuoka et al. 2013; Lewis and Arrigo 2020), and tunings for antarctic waters account for lower $a_{\mathrm{CDOM}}(440)$ relative to C_a (Dierssen and Smith 2000). The latter is also in keeping with highly nonlinear formulations of OC algorithms, e.g., the number of power terms used in the polynomial model to fit C_a to ratios of R_{rs} is routinely four (Morel 2009; O'Reilly and Werdell 2019). Linearity and loglinearity of CDOM algorithms increases with increasing spectral separation of wavelengths (Hooker et al. 2020, 2021a; Houskeeper et al. 2021). The results herein suggest that differences in linearity correspond, in part, to differences in the separability of signals associated with spectral range."

- *Line 580: "aCDOM and Ca absorption" instead of "aCDOM and CDOM absorption"?*

Authors Response 42: The authors thank the reviewer for catching this mistake. The authors revise the text, as follows:

> "…confounding effects of spectral overlap in C_a and CDOM absorption…"

The authors thank Reviewer 2 for useful comments and suggestions, which helped the authors to improve the manuscript.

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