

## CC1: 'Comment on essd-2025-443', Elizabeth C Atwood, 22 Dec 2025

We would also like to thank you so much for your feedback and valuable comments. Our response and actions are listed below in blue.

### General comments:

Excellent overview in the Introduction, albeit with some specific comments below. The method shows good promise but I have some reservations, noted in Specific Comments below. The speculative other features of the data (§5) are not especially unique to this dataset. The provided dataset, while impressive, is not validated, which is mentioned in the manuscript and should not be forgotten by potential users (or in future references to this paper).

**Response:** Thank you. Especially regarding the question of validation, we would like to refer to our detailed responses to Reviewer #1 and our corresponding changes that include rough POC validation (for one water type) and explain difficulties of validation. Moreover, even though this end-to-end processing scheme is not yet published in detail or available code-wise, there are already some mentioned references that include validation, e.g. of  $R_{rs}$  (Hieronymi et al., 2023).

### Specific comments

L50-51: I don't see a result in either reference saying that precipitation can be a source alone for CDOM?

**Response:** The reference mentioned Kieber et al. (2006) states in the abstract: All rainwater samples contained chromophoric dissolved organic matter (CDOM) as well as fluorescent compounds. This is what we also observed in our rainwater samples at the open Atlantic Ocean.

**Changes:** We added another relevant literature review to the diverse CDOM sources, namely Nelson and Siegel (2013).

L52: Water movement in rivers and lakes would be in a different category to currents, should be explicitly included since your main point is to cover the limnological to the oceanographic.

**Changes:** We rephrased the sentence to: "Sediments are kept in suspension by water movement in rivers and lakes, or in shallow waters by currents, tides, and waves."

L71-72: It is the aim to cover all water areas uniformly and with sufficient data quality, not only of this study but of these other services, no matter that there do still exist areas for improvement. I suggest removing "Thus".

**Changes:** OK, thanks – done.

L77: Compromised when a single AC method optimized for a specific water type is used.

**Changes:** We have revised the sentence as suggested to clarify this limitation. The text now reads: "... a requirement often compromised when a single AC method optimized for a specific water type is used."

L78-79: What about Atwood et al (2024, doi: 10.3390/rs16173267), which focused precisely on transitional water systems? Spyros et al (2018, doi: 10.1002/lno.10674) also focused on coastal as well as inland waters.

**Changes:** We acknowledge the relevance of these studies regarding transitional and coastal/inland water classification. We have added citations to Atwood et al. (2024) and Spyros et al. (2018) in the specified sentence to explicitly credit their contributions to this

domain: “This approach is particularly valuable for capturing transitional waters (e.g., river plume or algal bloom fronts), as also highlighted in studies of coastal and inland systems (Spyrakos et al., 2018; Atwood et al., 2024), where optical properties vary non-linearly with constituent concentrations.”

L90-92: This is not as novel as it is being presented, such a system to continuously monitor from rivers, through coastal areas to the ocean has been demonstrated through the CERTO project.

**Changes:** We included a reference to the similar approach of the CERTO project and Atwood et al. (2024).

L113-116: This has good potential for large overrepresentation of more oceanic waters in the training dataset, thus skewing the cluster optimization results to be oriented on oceanic water conditions than the smaller by area transitional water systems.

**Response:** Here, we describe the sub-domain “coastal waters”. The distance to coast is comparable with the high-resolution coastal product in the Copernicus Marine Service. We only define a sub-region that corresponds to the product and the general term coastal waters. We perform OWT analysis everywhere, but specifically look into this masked region too. The data points within this mask are not used for OWT training or clustering. Bi and Hieronymi (2024) is based on simulated data (Bi et al., 2023) and includes all optical extremes. The dataset can be used to focus on transitional water systems and OWT weight distributions, which is currently not discussed.

L144-146: To cite a method for the current study in a manuscript that is still being prepared is questionable.

**Response:** This is true, but the lengthy and complex development of the end-to-end processing scheme is also not easily publishable. Different aspects are published, like ONNS and the new OWT scheme. The atmospheric correction is similar as the one in C2RCC, which misses a proper reference too, but is widely used by the community. We rephrased the section.

L155-156: What was the range of time offsets between S-3A and 3B? For coastal systems which are strongly tidal, a difference of over 45 min during the right tidal cycle can greatly change the water optical properties in a single location. This is less of a worry for the Baltic Sea, but certainly for the North Sea, in particular the English Channel. I question then what a mean pixel-reflectance value represents when taken from images at different times/tidal conditions for those coastal regions.

**Response:** This is exactly the kind of feedback we hope to receive from users of the dataset – thank you very much. The masking needs to be carefully refined, among other things to highlight potential influences of sun glint (which is currently not done) or to identify areas affected by tidal dynamics. The exact time offset depends on the region. For the entire region the time window is approximately three hours of data acquisition.

**Changes:** We included a reference to Sent et al. (2025) on the importance of tides for ocean colour applications to estuaries. “So far, potential effects of tidal dynamics, particularly relevant in regions such as the Bristol Channel or the Elbe River estuary, have not been accounted for in the merging, which may influence the products (Sent et al., 2025).”

L173: With regard to the SST assumption for same latitude, not including elevation probably makes less of a difference over the study area, but in the next sentence you mention Dead Sea and Great Salt Lake. Surely on a global scale it would further be important to include additional

aspects (like elevation, distance from coast, etc) to estimate freshwater system SST, other than just latitude.

**Response:** The climatology used is under revision too, also because of your legitimate concerns. The climatological data assist the processing and in future more the flagging too, e.g. on tides. Nevertheless, improved bridging between the different Copernicus Services would also be desirable in this regard.

L283-284: The c-mean algorithm provides membership values to all classes, not a subset as suggested with “three to six classes usually contributing”. If you aren’t providing memberships to all classes, how do you determine what subset of classes to calculate memberships for?

**Response:** You are correct that the algorithm calculates membership values for all defined classes. Our statement referred to the practical observation that, for any given spectrum, typically only three to six classes exhibit significant membership probabilities (e.g.,  $> 10e-4$ ), while the remaining contributions are mathematically non-zero but negligible.

**Changes:** We have revised the text to be precise: “... During the OWT analysis of the reflectance, weights are assigned to all defined classes, although typically only three to six classes contribute significantly.” Please also note that a new section and figure have been included according the comments of reviewer #2.

L285-286: A minimum requirement for total membership of 0.0001? I think this written differently than it was meant, that would be impossibly low for a summed membership even if unbounded. I also don’t find “0.0001” in Hieronymi et al (2023a). I am going to assume this is meant a minimum threshold a valid dominant OWT membership, and I would argue this threshold is far too low. For bounded memberships, i.e. summing to 1, a good rule of thumb for minimum membership definition is  $1/C$  where  $C$  is the total number of OWT classes. This would occur if a point is assigned equal membership to all clusters, thus suggesting it does not belong well to any cluster. This rule of course deviates in the case of unbounded memberships that can sum to more or less than 1, as in Moore et al. (2001), Jackson et al. (2017) and Bi & Hieronymi (2024). But it is argued in Bi & Hieronymi (2024) that memberships should still sum to close to 1 if there is no redundancy or underrepresentation in the classification results. Thus being somewhere close to  $1/C$  threshold should still be advisable, which for the Bi & Hieronymi (2024) OWT class set with 10 classes, would be 0.1. Thus the threshold of 0.0001 seems unreasonably low to me. This point also relates to Fig. 12 and conclusions made therefrom.

**Response:** The reviewer is correct that for standard Fuzzy C-Means where memberships sum to 1, a threshold of 0.0001 would be meaningless. However, our method (Bi and Hieronymi, 2024) follows the approach of Moore et al. (2001), where individual class memberships represent probabilities based on the Mahalanobis distance. These are unbounded and their sum ( $U_{tot}$ ) indicates the overall similarity of the spectrum to the training dataset.

Here,  $U_{tot}$  acts as a “novelty detector” or outlier index. A threshold of  $1/C$  (0.1) would be appropriate for identifying ambiguous classifications in a closed set, but for outlier detection in our probabilistic framework, it would be too restrictive and exclude valid waters that deviate slightly from the class centroids. The threshold of  $10e-4$  is empirically chosen to flag only extreme outliers (e.g., severe glint, clouds, or non-water targets). This specific threshold value is documented in Table 3 of Hieronymi et al. (2023a) and on page 6 of Hieronymi et al. (2017).

**Changes:** We have added these references to the text for clarity: “The total membership serves as an indicator of the quality of the classifiability; a minimum requirement of 0.0001 is often used (e.g. Moore et al., 2001; Hieronymi et al., 2017, 2023a).”

L343-345: High variability of OWT class could come from other aspects besides shallow water and visible seafloor – unless that is also changing greatly? This variability could also be due to a location in a narrow water connection between to large water bodies. This also relates to the conclusion on L389 regarding using OWT classes as a mask for optically shallow water areas – is this supposed to follow over the high variability in OWT class signal?

**Response:** The main point here is that up to now, we have no real handle to mask out optically shallow water. However, in case of the island mentioned (or coral island in the ocean), surrounding water should be comparable. Comparisons with high resolution Sentinel-2 images show sandy bottom effects, partly with dark sea grass areas that cause different OWT allocation. This is also visible on some lake boundaries. During the year, adjacency effects may also occur or change with land cover (up to now assumed to be small for A4O) or sub-pixel contamination of growing plants may interfere, which could cause OWT variability. These points are already mentioned.

L360-361: Point well taken that low optical variability over time is important for ground-truthing and SVC, but the point in the parentheses “but rather for clear waters” is confusing. Do you mean that only clearer waters are important for ground truth and SVC? I would argue that optically complex water, but with low variability, would also be important for these efforts so as to cover a larger portion of the full spectrum.

**Response:** We agree with the reviewer that low temporal variability is the primary requirement for reliable reference data. While operational SVC typically relies on oligotrophic waters (to minimize  $L_w$  contributions and isolate atmospheric path radiance), we agree that stable, optically complex waters are scientifically valuable. They are particularly critical for ground-truthing (validation) to assess algorithm performance across the full dynamic range of the sensor.

OWT technology offers the opportunity to apply SVC per water type and per product. But some classes cover extremes that occur in small areas (black lakes, OWT 7) or small-time scales like intense phytoplankton bloom (OWT 5b). Moreover, your mentioned point with tidal effects might be relevant, as mentioned in the Bristol Channel, with always dominating OWT 6. Adjacency effects, shallow water, high cloud cover (rainy areas, sensor pollution), etc. should be avoided.

**Changes:** We have revised the text to differentiate these needs while highlighting the importance of stability for both. Revised text: “... For ground-truthing and definition of system vicarious calibration (SVC) gains, low optical variability over time is more important than water clarity alone. While SVC is traditionally performed in clear waters, stable optically complex waters are essential for validating algorithms and ground-truthing across the full spectral range. OWT technology provides the opportunity to apply SVC on a per-water-type and per-product basis.”

L447-449: It is at the moment speculative if OWT serve to better characterize aquatic carbon, including the example OWT 3b bloom, and this should be phrased accordingly.

**Response:** In fact, OWT narrows down ranges of water constituents and covariances of them. In the example with POC, there are linear contributions by plankton and detritus with different weight. Separation of both is essential for the magnitude of POC. Moreover, we can apply OWT-specific biogeo-optical relationships like for POC and DOC. The sources of DOC can be different in the diverse aquatic environments.

**Changes:** We reformulated “Optical water types have the potential to support improved characterization of aquatic carbon.”

L504-506: Mélin & Vantrepotte (2015) and Spyarakos et al. (2018) both focus specifically on coastal/transitional water systems, thus your conclusion is not fully supported. Also a critique that 17 classes may be too many simply on the basis of lacking in-situ data is not a very strong argument.

**Response:** We accept the reviewer’s correction. We acknowledge that the cited frameworks (e.g., Mélin & Vantrepotte, 2015; Spyarakos et al., 2018) indeed cover coastal and transitional waters. Regarding the number of classes, our argument was intended to address the statistical robustness of the validation process rather than the availability of data per se. Dividing limited in-situ matchups into a high number of fine-scale classes (e.g., 17) often results in insufficient sample sizes for reliable performance assessment per class. We have revised the text to correct the description of previous studies and clarify this motivation.

**Changes:** Revised text: “... Alternatively, other OWT frameworks can serve as a basis (e.g. Moore et al., 2001; Vantrepotte et al., 2012; Moore et al., 2014; Mélin and Vantrepotte, 2015; Jackson et al., 2017; Spyarakos et al., 2018; Bi et al., 2021; Atwood et al., 2024). However, some of these frameworks differentiate a large number of optical classes (e.g., up to 17). While scientifically rigorous, such high granularity can be challenging for operational validation, where a more consolidated set of classes is advantageous to ensure sufficient matchup density for robust statistical assessment of each water type.”

## Technical corrections

L55: The sentence starting here rather belongs thematically to the next paragraph.

**Changes:** A paragraph has been added here.

L100-101: You should indicate the location of Glasgow in Fig 1 if you reference it in the text. Same goes for the Elbe River catchment.

**Changes:** In response to another suggestion of reviewer #2, Fig. 1 now contains labels of all mentioned areas. Mentioning Glasgow as location has been removed.

L130: What do the various boxes (white or red) represent? This is not explained in the figure caption.

**Changes:** The boxes of individual scenes (white) and of the region of interest (red) have been explained in the figure caption. Moreover, Fig. 2 contains now a workflow.

L184: Suggested rewording for clarity: “Products from climatologies and their derivatives, such as white cap fraction, refer...”

**Changes:** Thank you, included.

L200: The first three parameters (OWT\_AVW, OWT\_Area, OWT\_NDI) are rather spectral curve characteristics directly from the Rrs, that are not dependent on output from an OWT classification? And OWT\_index, is this the dominant OWT class?

**Response:** The optical variables are part of the OWT classification. Index is indeed for the class with maximum membership.

**Changes:** “Parameters associated with the optical water type classification”.

L278: Is the AVW meant from Vandermeulen et al 2020? Then this shouldn't be mixed up with a normal weighted mean, better to change to “weighted harmonic mean” so this remains clear.

**Response:** The hyperspectral AVW in Vandermeulen et al. 2020 is calculated for the range 400–700 nm, our AVW refers to 400 to 800 nm to include hyper-eutrophic cases.

**Changes:** In response to reviewer #2, we introduced the OWT framework with a separate section and overview figure and rephrased this content.

L560: Remove the either “to” or “must”, incorrect with both.

**Changes:** Thanks, we removed “to”.

## References:

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