RC1: 'Comment on essd-2025-443', Anonymous Referee #1, 06 Nov 2025

We would like to thank you very much for reviewing our work and for your detailed comments. We will endeavour to incorporate your comments into the manuscript, primarily with a view to clarifying the discussion.

But first, we would like to comment on the main comment on the issue of validation, which all three reviewers found lacking. Working on an end-to-end processor for satellite imagery is very complex and time-consuming, it involves an atmosphere and a water component with strong interdependencies. For this reason, it has become apparent that the entire system should be considered for optimisation, also to develop appropriate flags. There are five fundamentally different data groups that need to be validated: meteorological (wind, solar irradiation), oceanographic (water temperature and salinity), apparent optical properties (R_{rs}, K_d, K_u, *FU*), inherent optical properties, and concentrations of water constituents - each sub-parameter has its own measurement method and error acceptance (e.g. IOCCG report on uncertainties, 2019). Furthermore, measurement methods encounter (undefined) limitations when used in different optical water types, e.g. R_{rs} measurements below or above water in clear or very turbid water. The call for product validation is justified, but it cannot be realised in a simple and compact manner in this paper. With this work, we aim to explain the fundamental assumptions, methods, and processing steps using a test dataset (and a scientific question about optical complexity of our region of interest) to also enable user feedback and, thus, create a citable reference to the community.

In fact, some of the products have already been compared with in situ data in the mentioned regional studies, with A4O-ONNS performing unsatisfactorily in some cases. The focus of the analyses in this article refers to remote-sensing reflectance in 14 out of 16 spectral bands, which serve as the basis for OWT analysis. In this regard, we would like to refer to the study by Hieronymi et al. (2023), in which R_{rs} from A4O was compared with in-situ data, particularly in comparison with the established atmospheric correction methods IPF, C2RCC, POLYMER, and Acolite. The comparison, e.g. here in Fig. 4 from their publication, also underlines the importance of flags for valid pixel expression. For example, in the standard AC of OLCI (IPF), large areas are conservatively flagged out, e.g. in sun glint (albeit the results may actually look good). Other methods such as A4O have no restrictions here so far; this alone results in significantly more possible matchups. In the processing currently under discussion, results from high sun glint areas are also incorporated into the Level-3 daily mean values. In preliminary tests, we have not found excessive deviations, but the test dataset serves to precisely analyse products and to define the valid pixel expression. For monitoring of the land-sea transition, the fundamental provision of classifiable R_{rs} spectra for all defined water types is crucial, and this is where A4O offers clear advantages. To underpin this, we would like to draw attention to Fig. S10 from the Supporting Information for Bi and Hieronymi (2024) in comparison with Fig. 12 of our article.

In fact, we are currently working on another publication that compiles all available R_{rs} measurements from the same region and time to perform validation of this dataset. That said, the data is very diverse from AERONET-OC or WATERHYPERNET stations, ship validation campaigns, autonomous ferry ship measurements, and measurements taken above or below water. Much of the available data does not meet *Fiducial Reference Measurements* quality requirements, and comparative values are not available for all water types. Describing these methods and their differences is complex and lengthy, and beyond the scope of this paper here. Please also note that measurement uncertainties for R_{rs} close to zero are very high, i.e. generally in the NIR, but also in the blue at higher CDOM concentrations, this limits meaningful validation for the bands. We would therefore suggest that the references to previous validation studies be highlighted more clearly in the manuscript.

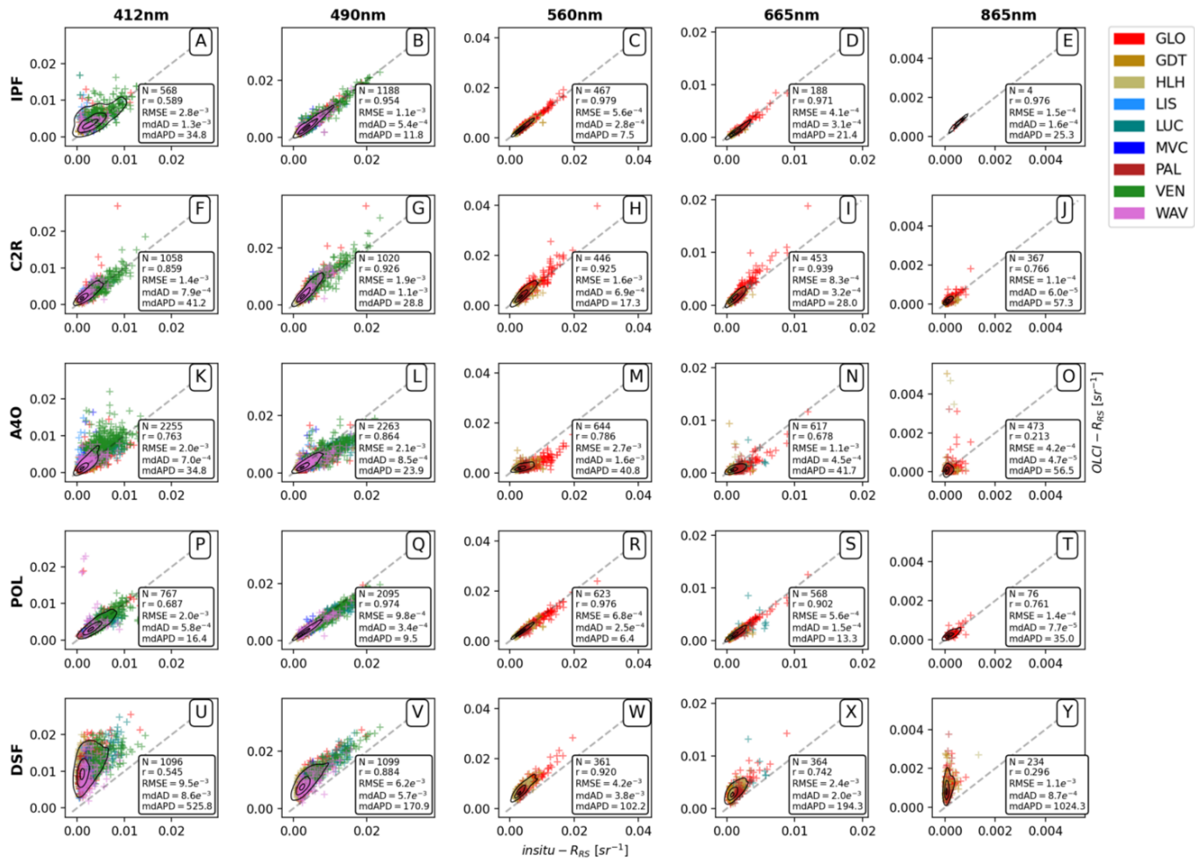


Figure 4 from Hieronymi et al. (2023) showing a comparison of satellite-derived R_{rs} with AERONET-OC in situ data for OLCI bands at 412, 490, 560, 665 and 865 nm for IPF (A–E), C2RCC (F–J), A4O (K–O), POLYMER (P–T), and ACOLITE-DSF (U-Y). The colors represent different stations. The contours indicate the density distribution. The different numbers of matchups (*N*) are mainly due to method-specific flagging and the spatial homogeneity criterion per band.

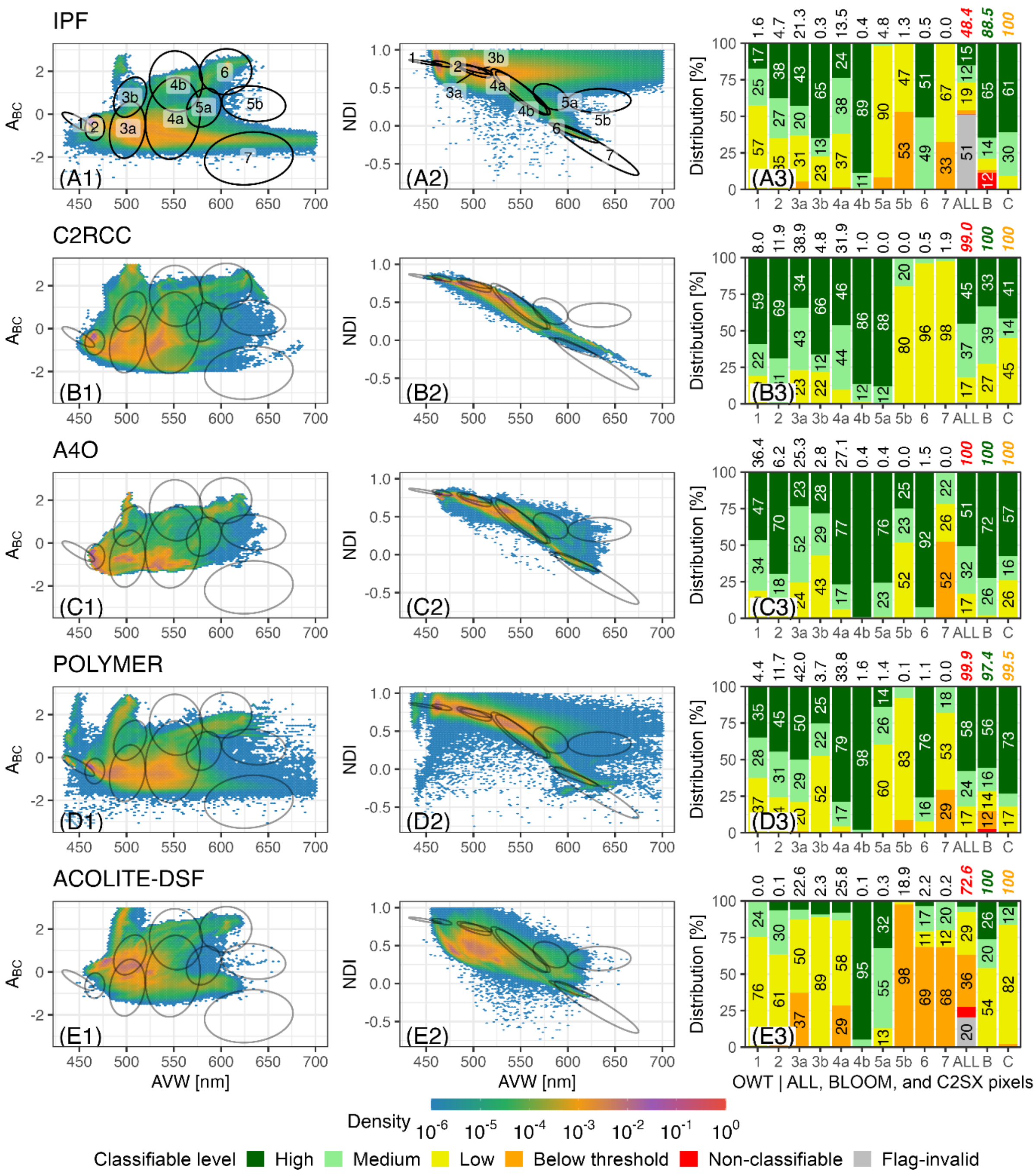
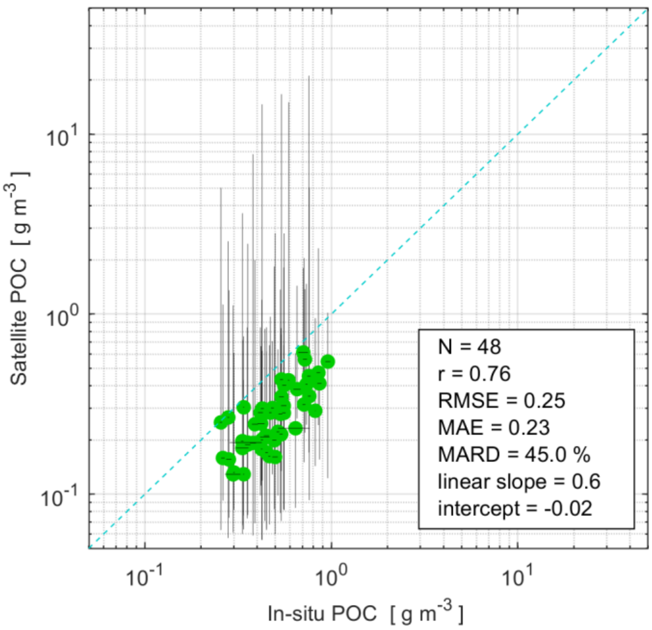


Figure S10 from the Supporting Information for Bi and Hieronymi (2024). It shows classifiability of R_{rs} from five atmospheric correction methods (including A4O, C1-C3) based on ten diverse OLCI test scenes.

The only water parameter really discussed in the article is particulate organic carbon concentration. We therefore suggest using this parameter to describe the complexity of validation and adding the following section:

“There is only very little measured and uncertainty-characterized validation data available for the same region and time. From a validation campaign with *RV Alkor* (AL597) in July 2023 in the Baltic Sea *POC* measurements are available with concentrations varying between 0.25 to 1 g m^{-3} (N = 48). The related determination errors were generally low (1-5 %), but in few cases up to 20 % (Hieronymi et al., 2023b; Novak & Röttgers, 2026). Based on both measured and satellite-derived reflectance, the waters during all these measurements were assigned to just one optical water type, namely OWT 4a. Nevertheless, there are considerable small-scale spatial variations, often caused by the occurrence of large cyanobacteria colonies. Standard matchup criteria require a narrow time window and spatial homogeneity, but cloud cover also limits the amount of available comparison data. To estimate retrieval performance, we use all measurement points and corresponding satellite observations for the entire month of July 2023. Figure 15 shows a comparison of *POC* values from satellite observations with median of values from 3x3 pixels using a homogeneity criterion and cloud-free conditions within 5x5 pixels. The error bars for satellite-derived *POC* represent the minima and maxima of the mean values for the month and indicate that the values can vary by an order of magnitude, which is often related to unrecognized cloud artefacts (typically resulting in higher *POC* concentrations). This shows that rigorous system-wide flagging needs to be improved. However, Pearson's correlation coefficient shows a strong positive relationship ($r = 0.76$). The absolute root-mean-square error (*RMSE*) is 0.25, the mean absolute error (*MAE*) is 0.23, and the median absolute relative difference (like in Smith et al., 2018) (*MARD*) is 45 %. Linear regression yields a slope of 0.6 and an intercept close to zero; *POC* is therefore rather underestimated with considerable variability. However, we argue that explicit uncertainty characterization is also the dimension of high-quality earth observation data. This rough comparison (for one water type) is similar to the other OC products in the dataset and shows that there is still substantial need for improvement of the end-to-end processor. However, it also shows the opportunities for OWT-specific adaptation of IOP-concentration relationships and application of system vicarious calibration."



New Fig. 15: Comparison of particulate organic carbon measured in-situ from water in the Baltic Sea against satellite estimates from the same month (July 2023). The horizontal error bars of the in situ *POC* concentrations represent the standard errors from the determination. Vertical lines show the variation in median values in 3x3 pixels of the satellite images over the entire month. The 1:1 line is shown as a dotted line.

RC1: The manuscript documents a daily aggregated, Level-3 dataset produced by merging all available Sentinel-3 OLCI observations from both S3A and S3B overpasses for each day across the North Sea and Baltic Sea during June to September 2023. The processing chain uses the

A4O atmospheric correction followed by the ONNS neural network water processor. The data product includes remote-sensing reflectance at 16 OLCI bands, a suite of inherent optical properties, concentrations such as chlorophyll, TSM, DOC and POC derived from IOPs, the Forel-Ule color index, optical water type classifications, and several quality and context flags including cloud masks, adjacency risk, glint risk, bright pixel flags, and a whitecap fraction parameterization. The paper states that this is a prototype release, that no full validation of the many variables is provided here, and that the code will only be released in the medium term. The archived dataset is now at WDCC with a DOI, CC-BY 4.0 license, and a variables document.

The dataset targets a well known gap in ocean color for optically complex waters at the land sea interface where standard processing is often limited. Using both S3A and S3B improves daily spatial coverage, and a single pipeline across inland and coastal waters is attractive for monitoring and for synoptic biogeochemical analyses. Coupling an OWT framework to both atmospheric correction and water property retrieval is methodologically coherent, and providing OWT outputs alongside geophysical variables is useful for quality screening and for science use. As an ESSD submission, the core value is the accessible, gridded Level-3 product with metadata, DOIs, and a usage context. These positive aspects are clear in the paper.

Response: Thank you for recognising the value of our work and highlighting its potential.

The manuscript explicitly states that publication of the code is only planned in the medium term and does not include a Code availability section. ESSD allows data-only descriptions, yet it strongly encourages deposition of software and algorithms in FAIR repositories and requires a Code availability section when code is part of the work. For complex EO processing pipelines that strongly condition the resulting data, ESSD policy emphasizes transparency and reproducibility as core principles. In its current form, the work falls short of these expectations because independent users cannot reproduce the dataset or verify implementation details of A4O or the specific ONNS configuration used. At minimum, a versioned, citable container image or repository with the exact A4O and ONNS code paths, trained weights, and runtime environment is needed, together with a Code availability section that points to those DOIs.

Response: Thank you for your comment – we agree in principle. There are several aspects to consider here. Firstly, it is primarily about a dataset that we have created with great effort and many days of runtime; that is a value in itself. We have cited several sources with alternative processing methods (section 8.3), some of which are based on the same original data; in this respect, comparisons are possible and transparency is guaranteed. Please also note that many of the Level-2 or Level-3 methods mentioned are not freely available, including the standard processing by EUMETSAT. We are actively working on improving the technology readiness level of the end-to-end processor. This paper serves to document the basic concept, albeit in an intermediate stage, where the AC, OWT, water components and flagging have not yet been adapted. The development of this complex system is dynamic, and substantial changes are foreseeable. We are currently unable to publish the code for the processing chain as it stands, but we will prioritise after your feedback (depending on funding).

Please also note that this article primarily deals with the scientific question of the optical complexity of the North Sea-Baltic Sea region. As described in Hieronymi et al. (2023), available atmospheric corrections are insufficient to represent the complexity across different OWT frameworks, because they do not provide R_{rs} of some defined classes, i.e. they do not function well for all waters. Based on the findings of this study, a new OWT framework (Bi and Hieronymi, 2024) was created, its code is freely available (https://github.com/bishun945/pyOWT). As illustrated in the figure above from their publication, A4O generates R_{rs} spectra with the widest optical variance and the best classifiability. In principle, however, we could have clarified the question of optical complexity of the region using any other AC method; the uncertainties were explained in the article, but the results should be fundamentally comparable.

Changes: We include a reference to the OWT code, which can be used to reproduce the results of this study or can be applied to other atmospheric correction methods or satellite data.

The retrieval chain uses neural networks and an AC method. Small choices in training data, preprocessing, and band handling materially change IOPs and derived concentrations. Without the code or at least a fully specified ATBD with the exact trained model artifacts, an independent group cannot regenerate the L3 product from S3 Level-1 data. That limits reuse and undermines the central ESSD promise of transparent, reusable data products.

Response: As already noted, providing codes and training data is a complex task that is not feasible for this publication. The data used to train the neural networks – and this is only one aspect of the overall system – consists mainly of results from extensive solar radiative transport simulations in the atmosphere and in water. Processing the large amounts of data would be a huge task, but publication will be considered in the future – now, it cannot be made available. We have also written that there will be further adjustments regarding OWT-specific water NNs. Biogeo-optical modelling has developed significantly, especially with regard to assumptions for particulate scattering (Bi et al., 2023).

We would also like to refer back to our discussion on the dataset. It offers a wide range of parameters and links for further application of all kinds of "algorithms", such as deriving chlorophyll concentration from reflectance or determining Secchi depth from K_d. One could therefore apply any (!) *Chl* algorithm and compare it with our *Chl* estimate. In principle, one could even apply a different atmospheric correction and subsequent water algorithms to our dataset, as it contains top-of-atmosphere reflectance too. We have explicitly placed great emphasis on reusability, transparency, and connectivity of the dataset.

The ONNS basis is documented in Frontiers in Marine Science and is citable, which is a strength. However, the present chain departs from the 2017 ONNS in key ways. The paper indicates that concentrations now come from ONNS-derived IOPs rather than directly from class-specific networks, and that the OWT scheme used here is the newer Bi and Hieronymi framework. Those choices are reasonable, yet they change the forward model and error propagation, so they must be documented with enough specificity to be reproducible. The A4O method has been compared against other ACs, but a full methodological description plus code or trained models are still not publicly archived.

Response: We acknowledge that publishing a dataset without the full, open-source processing chain presents challenges for direct reproducibility. However, we argue that the primary contribution of this work lies in the unique coverage and quality of the generated products, particularly in optically complex waters where standard processors often fail. This dataset provides a critical benchmark that allows the community to evaluate the results, even while the full processing tool remains under development.

Regarding the selection of output variables, our approach mirrors established operational practices. For instance, standard Sentinel-3 OLCI Level-2 products provide both CHL_OC4ME (semi-analytical) and CHL_NN (neural network) estimates. This is not an inconsistency, but a recognition that different algorithms rely on different assumptions, and their performance varies depending on the optical water type. By providing our specific ONNS-derived IOPs and concentrations alongside standard products, we ensure transparency in our method's performance. This approach allows users to evaluate the "fitness for purpose" of different algorithms for their specific regions of interest and to report which product yields the most accurate representation. Therefore, this dataset serves as a necessary intermediate step to enable such comparative studies and user feedback, which are essential for the future harmonization of the end-to-end processor.

The manuscript is explicit that it does not perform a full validation of the many variables. For an ESSD data description that is acceptable only if adequate demonstration of fitness for purpose is provided and if uncertainties and quality information are delivered in a way that users can apply. Here, the validation evidence is mostly qualitative, which is a weakness. The paper even notes a possibly erroneous blueward tendency of A4O in some conditions and that reflectance magnitude is often underestimated, which is significant because Rrs is the driver for all IOP and concentration products. Users need at least some quantitative, OWT-stratified matchup statistics versus in situ Rrs and against IOP and concentration measurements, with uncertainty budgets that follow accepted EO data record practice. A concise validation plan can be staged, but the first ESSD version requires some validation.

Response: Please note our comment at the beginning and the difficulties involved in carrying out comprehensive validation. However, beyond standardised product validation, which is indeed lacking, we would like to draw attention to the detailed OWT analysis in the ESSD manuscript. This demonstrates precisely the fitness for purpose in a way that classic validation does not. The above Fig. S10 from Bi and Hieronymi (2024) shows the ability of five atmospheric correction methods for OLCI to produce certain spectral shapes and magnitudes of R_{rs}. Compared to standard AC (IPF collection 3), A4O never outputs negative reflectance, is not initially flagged as invalid in high sun glint, and induces less spatial noise, and thus generates "valid" results for an image area twice as large – with generally better classifiability, i.e. accepted R_{rs} spectra (Hieronymi et al., 2023). IPF has for example problems in cases with high algae biomass (OWT 5a&b) or high *CDOM* concentrations (OWT 7), which would be particularly important for the Baltic Sea and inland waters. Figure 12 from our manuscript shows that R_{rs} from A4O can be well-classified in 99.68% of the cases in this region. In the absence of dense in-situ networks, such spectral consistency and classifiability serve as critical proxy metrics for data quality. These are arguments that prove that A4O has a better fitness for purpose for this optically complex region than the standard atmospheric correction, which is considered validated. The uncertainties of the classification were outlined and reflected in your remarks; improving performance is a subject for ongoing research. Once again, we would like to point out that with this published dataset and its description in ESSD, we can now carry out careful OWT-specific validation of all 73 products (where available).

Changes: We propose further elaborating on the aspect of fitness for purpose and formulating a clearer validation plan.

The variables list in the paper and on WDCC is helpful, but several names and units would benefit from alignment with existing community standards. For NetCDF, CF conventions recommend using standard_name attributes where possible and consistent units and descriptive long_name fields. For ocean color, ESA CCI and NASA ocean color products provide a de facto vocabulary, for example RRS for remote-sensing reflectance, CHLOR_A for chlorophyll, K_490 for diffuse attenuation at 490 nm, APH for phytoplankton absorption, ADG for CDOM-plus-detritus absorption, and BBP for particulate backscattering. The present ONNS variable names such as ONNS_a_g_440, ONNS_b_p_510, and the use of the term Gelbstoff for

CDOM are understandable in context but may confuse users who expect CF-style names and common ocean color acronyms.

Response: The naming of variables is a serious problem, where we spend much time trying to solve it. Within the mentioned sources in Section 8.3, the following products for chlorophyll concentration based on OLCI-estimates are used: CHL_OC4ME, CHL_NN, Chl-a, Chlorophyll-a, chlor-a, chla_mean, chl, CHL, etc. Even for such common parameters as chlorophyll concentration, each source uses its own terminology. A genuine standard, e.g. at IOCCG level, would be desirable. Also, the use of "K_490 for diffuse attenuation at 490 nm" is too unspecific, at least Kd_490 with *d* for *downwelling* is useful. We feel that many "CF style names" are not precise enough defined in our field and cross-cutting limnology and oceanography. Many definitions are misleading https://cfconventions.org/Data/cf-standard-names/current/build/cf-standard-name-table.html (e.g. search for chlorophyll) - none of the standard names refer to fresh water for example. Our naming of variables is guided by the usage of the software Hydrolight and Mobley (1995). The names may not be ideal, but they follow a structure that we consider reasonable, e.g. naming the concentration and the underlying method at the same time, as in CHL_OC4ME. With IOP_Chl, we emphasise that the concentration is derived from the IOPs and not directly from a neural network, for example.

Changes: We include a discussion element for future initiatives.

On reflectance terminology, the manuscript lists A4O_Rrs_n as normalized remote-sensing reflectance. In ocean color there is potential confusion between fully normalized water-leaving radiance nLw, remote-sensing reflectance Rrs, and various normalization schemes. The paper should define exactly what normalization means in A4O, how it differs from standard Rrs, and why the units remain sr-1. That definition should also be embedded in the NetCDF metadata so that users do not misinterpret the quantity.

Response: Here you address aspects that also illustrate why the validation of the diverse product groups cannot be dealt with on a single page, but rather deserves dedicated, complex studies. The atmospheric correction A4O approximates a remote-sensing reflectance (bottom-of-atmosphere) from directional radiance and transformed reflectance at the top-of-atmosphere under the following characteristics: 1) The sun's position and viewing angle are assumed to be exactly perpendicular ($\theta_S = 0°$, $\theta_V = 0°$), 2) wind influences are set at 5 m/s, which is a standard assumption for water algorithms, and 3) R_{rs} is free from the effects of whitecaps and air bubbles in the water. These are harmonised angles and environmental conditions to enable global comparability and maximise the exploitation of satellite data, including in sunglint conditions. The disadvantages are that measured reflectance must be modified quite significantly to obtain fully normalised reflectance and to ensure comparable conditions, and that these modifications depend on the optical water types. The uncertainties of the approach and assumptions are reasons why sensitivity tests based on such a dataset are necessary.

Changes: The precise definition of the delivered R_{rs} and the boundary conditions are integrated.

The provision of flags is welcome, including cloud masks, cloud risk near edges, adjacency, glint risk, bright pixels, and a special flag for very high biomass or floating algae. The inclusion of a whitecap fraction parameter (A4O_A_wc) is scientifically useful because whitecaps increase broadband water-leaving signal and can bias retrievals if not handled. The whitecap parameterization is cited to satellite-based work, which is appropriate. What is missing is a clear, file-embedded description of how users should combine these flags for robust quality screening and what the recommended filters are for computing spatial or temporal aggregates.

Given that the paper acknowledges artifacts near clouds and adjacency and a blueward bias in some regions, the dataset should come with a documented, conservative quality mask and a short tutorial for users.

Response: Good point. The dataset is intended to be used to provide better recommendations for flags. Some masks can be regarded as independent parameters, e.g. cloud cover and floating algae, which also detects Sargassum, for example. Masks should always be seen in their spatial context; in the Baltic Sea, floating algae also marks intense Cyanobacteria blooms with a high Rrs-NIR signal, where the basic assumptions can be problematic if one cannot see into the water but estimates the concentration in volume. With regard to the whitecap fraction, it is a feature of A4O that these effects are removed so that subsequent water-retrieval is not biased. In this respect, the specification serves not only to provide information on air-sea fluxes, but also to ensure transparency that potential influences have been removed.

Changes: Recommendations for using the flags are included.

The dataset is built from both Sentinel-3A and Sentinel-3B OLCI sensors merged to daily Level-3. That is effectively a dual-sensor product within a single mission. The title reads as derived from satellite data, which could be interpreted as multisensor across missions. The abstract clarifies that the source is Sentinel-3 OLCI, and the methods section explicitly states S3A and S3B. To avoid misunderstanding, I recommend reflecting the instrument in the title or at least stating prominently on first mention that this is an OLCI-only product that merges S3A and S3B.

Response: We focus on the scientific question of the optical complexity of the region in order to provide a benchmark for the reliability and comparability of the algorithms used, e.g. for the Copernicus Marine or Land Services. This could also be estimated from other satellite data (MODIS, VIIRS, PACE, multi-sensor merged, or from diverse Copernicus Services) or widely distributed in situ reflectance measurements. Similar spatial patterns are also shown in Mélin and Vantrepotte (2025) based on SeaWiFS, for example. Sentinel-3 OLCI is a well-suited platform for this, but we would not want to over-emphasise this in the title.

Summary

ESSD requires a Data availability section and encourages authors to archive software and provide a Code availability section. The paper satisfies data availability through the WDCC DOI. It does not yet satisfy the spirit of ESSD reproducibility for algorithmic data products, because the code is not accessible and the AC is not documented at the ATBD level. ESSD explicitly invites authors to deposit code and even supports literate programming submissions to maximize transparency. This manuscript should follow that guidance for acceptance. The dataset fills a scientific gap but the present paper is not ready for acceptance because reproducibility and quantitative validation are not yet sufficient, and because naming, terminology, and user guidance need revision for broad reuse. If the authors release the processing code, add validation and/or uncertainty descriptions, align variable metadata with CF and common ocean color practice, clarify scope, and document flagging rules, I would recommend acceptance after those changes.

Response: In this paper, we have interwoven two aspects: 1) description of a satellite data processing chain with A4O-ONNS and 2) analysis of OWT in the region based on an A4O-ONNS dataset. The larger part is about OWT analysis, and with the suggestions of the other reviewers, it is growing even more. The OWT code is freely available. The OWT analysis can also be based on completely different data, as long as the methods used are fit for purpose. This has been demonstrated with the A4O atmospheric correction and OLCI data. Reproducing the underlying data set is indeed not yet possible for outsiders, but it would also involve a massive effort and, in our opinion, would not be necessary to clarify the scientific question addressed in the paper. We have openly communicated the further development steps of the overall algorithm in the document. However, we have also shown in our responses here how complex and complicated your demands would be. These questions cannot be answered in a few extra pages and are therefore out of scope for this work. We will document and validate the individual aspects of the processor separately, e.g. atmospheric correction and the corresponding R_{rs} as output. This requires a thorough understanding of optical water types, also to understand measurement errors. This also offers the possibility of targeted application of System Vicarious Calibration per OWT. Thus, we hope that our changes and exemplary comparisons with (relatively) few uncertainty-characterised measurements (of *POC*) will lead to acceptance of our work.

References:

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