Response to Reviewer #2

General Comments

This manuscript presents a global, monthly, three-dimensional chlorophyll-a (Chl-*a*) dataset for 2005–2025, reconstructed using a multimodal Profile-Surface Transformer (PST) framework. The framework combines BGC-Argo Chl-*a* profiles, Core-Argo temperature-salinity profiles, and MODIS satellite-derived surface Chl-*a* to estimate the vertical distribution of Chl-*a* from 10 to 500 m. The topic is timely and relevant to ESSD, as most existing global Chl-*a* products are largely limited to surface observations, whereas subsurface Chl-*a* structures are important for understanding phytoplankton biomass, primary production, carbon export, and ecosystem responses to climate change. The manuscript is generally clearly written, and the proposed dataset has the potential to become a useful community resource. However, I have several substantive concerns that should be addressed before publication. In particular, the uncertainty characterization of the final product remains limited, several key preprocessing and model-design choices are insufficiently documented, and some aspects of the reconstructed dataset require clearer evaluation and interpretation. I therefore recommend minor revision.

Really appreciate the reviewer for providing detailed and constructive suggestions that were very helpful for improving the manuscript. We have revised the manuscript accordingly, include renaming and revising Sect. 4.3 to better distinguish external validation from reliability diagnostics, adding RMSE, MAE, and bias for the final gridded product, providing interpolation and sampling-support diagnostics as ancillary variables in the NetCDF product, clarifying the use of corrected BGC-Argo Chl-*a* fields and fluorescence-related quality control, adding the explicit density-anomaly formulation, providing the full mathematical expressions for the depth-dependent gate and the composite loss function, clarifying the ship-based deep-background correction and temporal coverage of the external validation cruises, revising the SCM-depth interpretation, explicitly stating the log10-transformed modelling space, adding units to the Chl-*a* variable, and correcting the technical issues raised by the reviewer. Detailed point-by-point responses are provided below.

Specific Comments

1. Comment:

The uncertainty assessment of the final data product is currently insufficient. I checked the dataset provided through the repository link, and the final NetCDF files do not appear to include uncertainty-related variables. This limits users' ability to assess the reliability of the product across regions and time periods. Section 4.3 is entitled "Evaluation of the interpolated product and uncertainty analysis", yet the analyses presented mainly consist of comparisons against ship-based observations. This represents external validation of the gridded product rather than a comprehensive uncertainty assessment. In addition, only R and R2 are reported in this section. For consistency with Section 4.1, it would be preferable to additionally report RMSE, MAE, and bias.

Response:

We agree with the reviewer that the original wording of Section 4.3 overstated the scope of the uncertainty analysis. We have revised the title to "External validation and reliability diagnostics of the interpolated product" to more accurately describe its content. The revised section now distinguishes between external validation against independent ship-based observations and reliability diagnostics derived from interpolation and sampling-support information.

We have also added additional product-level validation metrics. In the revised manuscript, RMSE, MAE, and bias are reported in linear Chl-*a* space to quantify absolute errors in physical concentration units, while R and R^2 are reported in $\log_{10}$ Chl-*a* space to evaluate the consistency of relative variability across the broad dynamic range of Chl-*a*. The revised product-level validation results are RMSE = 0.23 mg m^{-3}, MAE = 0.079 mg m^{-3}, bias = −0.015 mg m^{-3}, R = 0.84, and R^2 = 0.63. We also revised the interpretation to state that the gridded product shows reasonably low absolute errors and remains broadly consistent with independent ship-based observations, while acknowledging the additional smoothing, scale-mismatch, and representativeness errors introduced by monthly gridding and spatial interpolation.

In addition, interpolation and sampling-support diagnostics have been added as ancillary variables in the NetCDF product to support user assessment of product reliability across regions, months, and depth levels.

2. Comment:

The authors mention in lines 359–363 that interpolation diagnostics were recorded, including the number of profiles used for interpolation, the proportion of missing values within the ocean domain, and the frequency of use of different interpolation radii, yet none of these diagnostics are actually presented anywhere in the manuscript. The sources of uncertainty in the final product, including model prediction errors, errors introduced by the spatial interpolation procedure, and the propagation of input data uncertainties, should be systematically evaluated and provided as ancillary variables within the NetCDF product.

Response:

Thanks for the great suggestion. We have revised Sect. 3.5 to provide a clearer and more complete description of the interpolation and sampling-support diagnostics recorded in the updated product, and revised the uncertainty-related discussion to explain how these diagnostics can be used as practical reliability indicators.

In the revised manuscript, we now clarify that the updated product includes not only the main reconstructed Chl-*a* field, but also coordinate variables, product attributes, interpolation parameters, time–depth-layer diagnostics, radius-usage diagnostics, and four-dimensional grid-cell-level interpolation-reliability diagnostics.

Specifically, the product includes the main variable chl_4d;

coordinate and grid variables time_ym, depth_profile, lat_grid, lon_grid, and grid_res;

product metadata including product_title, product_version, chl_units, chl_long_name, and chl_ancillary_variables;

and interpolation-parameter variables including method, r_list_km, good_n, min_n, nearest_fill, clip_by_percentile, clip_pct, and ocean_mask_used.

The product also includes time–depth-layer diagnostic variables, including n_points_used, n_profiles_used, nan_count_global, nan_count_ocean, ocean_coverage_after_nearest, adaptive_fail_counts_tz, nearest_fill_counts_tz, and final_fail_counts_tz.

Radius-usage diagnostics are provided through r_bins_km and r_usage_counts.

In addition, four-dimensional grid-cell-level interpolation-reliability diagnostics are included, namely interp_radius_km, interp_neighbor_count, adaptive_fail_before_nearest, nearest_fill_used, and nearest_fill_distance_km.

These diagnostics allow users to identify regions, months, and depth levels where the gridded Chl-*a* field is more strongly constrained by nearby profile observations and regions where it depends more heavily on larger interpolation radii, interpolation fallback behaviour, or nearest-neighbour filling. In general, grid cells supported by more nearby profiles and smaller adaptive radii can be regarded as more strongly observation-constrained, whereas regions requiring larger radii, adaptive-interpolation fallback, or nearest-neighbour filling should be interpreted with greater caution.

Accordingly, we have updated the released data product to **Chl3D_2005_2025_1deg_v2**, which is available at **https://doi.org/10.5281/zenodo.21219077**. These diagnostics are not intended to provide a full formal uncertainty decomposition of all possible error sources, but they provide practical reliability information related to observation density, interpolation support, adaptive-radius selection, interpolation fallback behaviour, nearest-neighbour filling dependence, ocean-domain coverage, and product completion. This revision makes the product more transparent and allows users to better evaluate data coverage and interpolation-related uncertainty when applying the dataset in regional or global analyses.

3. Comment:

The manuscript states that profiles passing both real-time and delayed-mode QC procedures were retained (line 166–167). It is unclear whether this means that only profiles that have undergone both RTQC and DMQC were used, or whether the dataset also includes RTQC-only profiles. If RTQC-only profiles were included, please report their approximate proportion and discuss whether differences between RTQC and DMQC data quality could affect the reconstruction. In addition, the manuscript does not clearly describe how fluorescence-specific corrections were handled prior to model training. This is important because different correction strategies can substantially affect Chl-*a* magnitudes, particularly in the upper ocean.

Response:

We thank the reviewer for pointing out this ambiguity. We agree that the original wording could be misinterpreted as indicating that RTQC/DMQC metadata fields were used as explicit filtering criteria. We have therefore revised Section 2.1 to describe the actual preprocessing workflow more accurately.

In the revised manuscript, we clarify that the corrected Chl-*a* field was extracted from each BGC-Argo profile file and used as the target variable for subsequent matching and model training. The extracted profiles were then further screened to remove profiles with obvious outliers, insufficient vertical sampling resolution, or unreliable pairing with physical profiles. After this profile-level quality-control procedure, 109,083 BGC-Argo Chl-*a* profiles were retained for model training, validation, and testing.

Accordingly, we no longer describe the retained profiles as being explicitly selected according to both RTQC and DMQC flags. Instead, the revised manuscript states that corrected BGC-Argo Chl-*a* fields were used, followed by additional profile-level quality screening. Because RTQC/DMQC metadata fields were not used as explicit selection variables in this preprocessing workflow, we do not define or report a separate RTQC-only proportion for the retained profile set. We also expanded the discussion of fluorescence-related quality control by citing previous studies that evaluated quality-control and correction procedures for BGC-Argo biogeochemical measurements and fluorescence-based Chl-*a* retrievals. This revision clarifies that the reconstruction framework was constrained by corrected and quality-screened BGC-Argo Chl-*a* fields rather than by uncorrected raw fluorescence values. We further note that fluorescence-specific correction and possible differences among BGC-Argo data-processing modes remain important sources of uncertainty in BGC-Argo-based Chl-*a* reconstruction, and we now discuss this more explicitly in the data and uncertainty-related sections.

4. Comment:

In lines 264–265, the manuscript mentions a "density-anomaly-related feature computed from temperature and salinity using a simplified equation-of-state formulation". Please provide the explicit formulation used for this calculation.

Response:

We agree and have added the explicit formulation in Section 3.3. The revised manuscript now defines the approximate density-anomaly feature as

$$\sigma_\rho = \rho_{simp}(T,S) - 1000, \quad (1)$$

where T and S denote temperature and salinity. The polynomial form used here follows the temperature–salinity dependence of the one-atmosphere seawater density equation, but was simplified for use as an auxiliary model input rather than as a full seawater-density calculation (Millero and Poisson, 1981; Fofonoff and Millard, 1983).

The simplified density term is calculated as

$$\rho_{simp}(T,S) = \rho_w(T) + A(T)S + B(T)S^{1.5}. \quad (2)$$

Here, $\rho_w(T)$, $A(T)$, and $B(T)$ are temperature-dependent polynomial terms.

For completeness, the polynomial coefficients are given below:

$$\rho_w(T) = 999.842594 + 6.793952 \times 10^{-2}T - 9.09529 \times 10^{-3}T^2 + 1.001685 \times 10^{-4}T^3 - 1.120083 \times 10^{-6}T^4 + 6.536332 \times 10^{-9}T^5,$$

$$A(T) = 8.24493 \times 10^{-1} - 4.0899 \times 10^{-3}T + 7.6438 \times 10^{-5}T^2 - 8.2467 \times 10^{-7}T^3 + 5.3875 \times 10^{-9}T^4,$$

$$B(T) = -5.72466 \times 10^{-3} + 1.0227 \times 10^{-4}T - 1.6546 \times 10^{-6}T^2.$$

This variable was used as an approximate, pressure-independent, physically informed predictor of water-mass density structure rather than as a full pressure-dependent potential-density estimate following EOS-80 or TEOS-10 conventions (Fofonoff and Millard, 1983; McDougall and Barker, 2011). This addition makes the density-anomaly-related input feature fully reproducible while avoiding overinterpretation of it as an exact seawater density calculation.

5. Comment:

The manuscript provides a detailed description of the PST model architecture. However, several design choices remain insufficiently explained. At line 290, the authors introduce an exponentially decaying depth-dependent gate to modulate the influence of satellite surface observations with depth. Please provide the functional form of this gate, clarify whether the decay rate is learned or prescribed, and assess the sensitivity of the reconstruction to this choice.

Response:

This is a very helpful suggestion. Section 3.3 is modified to provide the full formulation of the depth-dependent gate and to clarify which parameters are prescribed and which are learned. In the revised manuscript, the normalized depth index for the k-th depth level is defined as

$$z_k = \frac{k-1}{L-1}, \tag{3}$$

where L is the number of standard depth levels. The depth gate is then prescribed as

$$g(z_k) = \exp\left(-\frac{z_k}{\tau}\right), \quad \tau = 0.3. \tag{4}$$

We clarify that the exponential depth-decay function itself is prescribed, while the fine- and coarse-scale MODIS branch coefficients α_{fine} and α_{coarse} are initialized as 0.3 and optimized during training. Thus, the vertical decay scale τ is not learned, whereas the relative strengths of the two MODIS attention branches are learned from the training data.

To assess the sensitivity of the reconstruction to this prescribed decay scale, we conducted additional experiments using alternative τ values and a no-gate configuration. The results are summarized in Table R1. Across all tested settings, the performance differences were very small. RMSE varied only from 0.2250 to 0.2254, MAE from 0.1580 to 0.1585, and $R^2$from 0.8919 to 0.8922. These results indicate that the reconstruction was not highly sensitive to the exact prescribed value of τ. The default setting of τ=0.3 was retained because it provides a physically reasonable attenuation of surface satellite information with depth while maintaining stable reconstruction performance.

Table R1. Sensitivity of reconstruction performance to the prescribed depth-gate decay scale.

Experiment	Tau	N	RMSE	MAE	BIAS	R	R^2
no_gate	no_gate	816815	0.2254	0.1585	-0.0057	0.9444	0.8919
tau_0p2	0.2	816815	0.2252	0.1582	-0.0047	0.9445	0.8920
tau_op3_baseline	0.3	816815	0.2250	0.1580	-0.0089	0.9447	0.8922
tau_0p5	0.5	816815	0.2253	0.1584	-0.0058	0.9445	0.8919
tau_1pe	1.0	816815	0.2253	0.1583	-0.0106	0.9446	0.8919

6. Comment:

The model also uses a composite loss function that combines a depth-weighted masked mean squared error with a curvature-consistency term based on second-order vertical differences (lines 294–295). The exact formulation is not given. Please provide the full mathematical expression, including the relative weights of the two terms and the depth-weighting scheme.

Response:

We agree and have added the full mathematical expression of the composite loss function in Sect. 3.3. The revised manuscript now defines the total loss as

$$\mathcal{L} = \mathcal{L}_{MSE} + \lambda_{curv}\mathcal{L}_{curv}, \quad \lambda_{curv} = 0.2. \tag{5}$$

The masked MSE term is computed as

$$\mathcal{L}_{MSE} = \frac{\sum_{b=1}^{B}\sum_{k=1}^{L} m_{b,k} w_k \left(\hat{y}_{b,k} - y_{b,k}\right)^2}{\sum_{b=1}^{B}\sum_{k=1}^{L} m_{b,k} w_k + \epsilon}, \tag{6}$$

where the depth-dependent weight is prescribed as

$$w_k = 1 + 2\frac{k-1}{L-1}. \tag{7}$$

Thus, the weight increases linearly from 1 at the shallowest level to 3 at the deepest level. For the curvature-consistency term, the second-order vertical difference is defined as

$$D^2 y_{b,k} = \frac{y_{b,k+1} - 2y_{b,k} + y_{b,k-1}}{\Delta z^2}, \quad \Delta z = 10m. \tag{8}$$

The curvature loss is then computed as

$$\mathcal{L}_{curv} = \frac{\sum_{b=1}^{B}\sum_{k=2}^{L-1} m_{b,k-1} m_{b,k} m_{b,k+1} \left(D^2\,\hat{y}_{b,k} - D^2 y_{b,k}\right)^2}{\sum_{b=1}^{B}\sum_{k=2}^{L-1} m_{b,k-1} m_{b,k m_{b,k+1}} + \epsilon}. \tag{9}$$

In these equations, $\hat{y}_{b,k}$,kand $y_{b,k}$ denote the predicted and observed log10-transformed Chl-*a* values for sample b at depth level k, respectively; $m_{b,k}$ is the valid-observation mask; w_k is the depth-dependent weight; *B* is the batch size; *L* is the number of standard depth levels; and $\epsilon = 10^{-8}$ is used for numerical stability. These additions clarify the relative weighting of the two loss terms, the depth-weighting scheme, and the formulation of the curvature-consistency constraint.

7. Comment:

Regarding the deep-background correction applied to ship-based fluorescence profiles (lines 498–501), the authors state that a background value estimated below 300 m was subtracted from the original fluorescence-derived Chl-*a* values. Please specify how this background value was estimated. The external validation is based on 135 cruises, and Figure 4a shows their spatial distribution. Please also provide the temporal distribution of these cruises and indicate whether any years during 2005–2025 lack external validation data.

Response:

A new of Section 3.6, "Independent ship-based validation data and matching strategy," was added where the methodological details of ship-based preprocessing and matching was moved into this section. The revised text now specifies that, for each station profile within a cruise, valid raw fluorescence-derived Chl-*a* measurements below 300 m were used to estimate the deep-background value. When sufficient valid measurements were available below 300 m, the background value was estimated as the median of these deep measurements and subtracted from the original fluorescence-derived Chl-*a* values throughout the corresponding profile. This median-based correction was used to reduce the influence of deep fluorescence background drift and occasional deep spikes.

Figure 4a was updated to include an inset showing the annual distribution of retained validation cruises. In Section 4.2, we now report that, after cruise-level quality filtering, 135 cruises were retained, yielding 294,471 matched prediction–observation pairs. The retained validation samples provide temporal coverage for most of the reconstruction period, with matched samples available for 2005 and 2007–2024. No retained matched validation samples are available for 2006 or 2025 after the cruise-level filtering and matching procedure.

8. Comment:

The manuscript defines SCM depth as the depth of maximum Chl-*a* concentration within the 10–200 m range (line 639). However, as the authors themselves discuss earlier in the text and as clearly illustrated in Figure 5, Chl-*a* maxima in high-latitude regions with deep winter mixing often occur near the surface. In such cases, the vertical Chl-*a* profile may not exhibit a distinct subsurface peak, and the detected "maximum" simply reflects the surface-intensified distribution rather than a true subsurface chlorophyll maximum. Were these surface-dominated profiles excluded from the SCM analysis, or were they included in the statistics? If they were included, the reported SCM depths may conflate true subsurface maxima with surface-intensified profiles driven by different physical-biological mechanisms.

Response:

We agree with the reviewer that the diagnosed depth of maximum Chl-a does not always correspond to a distinct subsurface peak, because subsurface chlorophyll maximum layers may reflect multiple interacting ecological, optical, and physiological processes rather than a single profile type (Cullen, 2015). This issue is particularly relevant in high-latitude winter or strongly mixed regimes, where previous global analyses reported Chl-a maxima occurring within the mixed layer rather than as stable maxima below the mixed layer (Yasunaka et al., 2022). In such cases, the Chl-a maximum may occur near the surface and may reflect a surface-enhanced or upper-ocean maximum structure rather than a typical distinct SCM.

In our analysis, these surface-dominated profiles were not excluded by an additional SCM-occurrence criterion. Instead, SCM depth was used as an operational Chl-*a* maximum-depth diagnostic, defined as the depth of the maximum Chl-*a* concentration within the 10–200 m water column. We recognize that the previous wording may have led readers to interpret this diagnostic as a strict SCM/DCM occurrence classification. The relevant text was modified to clarify this point.

We further reviewed global and regional observational studies related to this issue. Previous studies have shown that stable subsurface Chl-a maxima are typically characteristic of tropical and subtropical stratified oceans, whereas surface-enhanced or mixed-layer maxima are less characteristic of low-latitude stratified open-ocean regions and are more commonly associated with high-latitude strongly mixed waters or winter deep-mixing conditions. This interpretation is consistent with the latitude-dependent structure reported in global BGC-Argo and Chl-a maximum-depth studies, such as Cornec et al. (2021) and Yasunaka et al. (2022).

To further evaluate the potential influence of this issue in our product, we also conducted a simple diagnostic analysis. Considering that maxima at relatively shallow depths may still represent true shallow SCMs, we did not use a fixed shallow-depth threshold to define surface-dominated profiles.

Instead, we adopted a more conservative criterion and used only cases in which the maximum occurred at the shallowest level as an indicator of potentially surface-dominated or near-surface maximum cases. The results show that these near-surface maximum cases are present in the global valid grid–month samples, but their spatial distribution is strongly latitudinally and regionally concentrated and they are not the dominant profile type in low-latitude tropical–subtropical stratified regions. Specifically, within 30°S–30°N, shallowest-level maxima account for only 1.85% of valid cases in this latitude band; meanwhile, only 2.90% of all shallowest-level maximum cases globally originate from 30°S–30°N. These results indicate that the surface-dominated cases noted by the reviewer are better interpreted as upper-ocean Chl-*a* maximum features under specific hydrographic conditions rather than as a widespread structure in low-latitude open-ocean regions.

Therefore, the inclusion of these cases is not expected to alter the main large-scale conclusions of our analysis. The focus of this study is not the occurrence frequency of true SCMs or DCMs, but the spatial distribution, seasonal variability, regional trends, and interannual variability of the diagnosed Chl-*a* maximum depth within the 10–200 m water column. The main patterns shown in Figs. 5 and 6, including deeper Chl-*a* maximum depths in tropical and subtropical oceans, shallower maxima in mid- to high-latitude regions, pronounced regional heterogeneity in SCM-depth trends, and a weak and statistically non-significant global-mean trend, remain valid. The potentially surface-dominated maxima mainly affect the interpretation of shallow diagnosed maxima in high-latitude or strongly mixed regimes, rather than the overall latitudinal structure or regional heterogeneity conclusions.

Accordingly, we have revised Sect. 5.5 and the related interpretations in Sect. 5, the Discussion, and the Conclusions. In the revised manuscript, SCM depth is explicitly described as an operational Chl-*a* maximum-depth diagnostic within the 10–200 m water column, rather than as an additional DCM-occurrence classification. We also clarify that shallow values in high-latitude winter or strongly mixed regimes should be interpreted as near-surface or upper-ocean Chl-*a* maximum depths rather than necessarily as distinct SCMs. The figures themselves were not changed, because they continue to show the diagnosed Chl-*a* maximum depth within 10–200 m; the main revision concerns the definition, interpretation, and wording of this diagnostic to avoid overinterpreting surface-dominated or near-surface maximum cases as strict true SCM/DCM occurrence.

9. Comment:

The model appears to operate in log-transformed Chl-*a* space (as suggested by the log-scale axes in Figure 3), but this is never explicitly stated. This should be clarified in the text. Additionally, the Chl-*a* variable in the downloadable NetCDF product lacks a units attribute, which should be added.

Response:

We agree and have clarified this in Sect. 3.3 and the validation sections. The revised manuscript now explicitly states that Chl-*a* concentrations were transformed to $\log_{10}$ space before model training to reduce the influence of their strong right-skewness and large dynamic range. Accordingly, the model output and loss function were defined in $\log_{10}$-transformed Chl-*a* space, and predicted values were back-transformed to linear Chl-*a* concentrations for generation of final gridded product.

We also revised the validation description to clarify that RMSE, MAE, and bias are reported in linear Chl-*a* space when physical concentration errors are evaluated, whereas R and R^2 are reported in log10 Chl-*a* space when relative variability across a broad concentration range is assessed. In addition, we have added the units attribute to the Chl-*a* variable in the NetCDF product. The Chl-*a* concentration variable is now provided with units of mg m^{-3}.

Technical Corrections

1. Comment:

Line 25: “integratessurface” should be corrected to “integrates surface”.

Response:

Thanks. Corrected.

2. Comment:

Line 76: “cycling. (Marañón et al., 2021).” should be corrected to “cycling (Marañón et al., 2021).”

Response:

Nice catch. Corrected.

3. Comment:

Table 1: The description of the spatial cross-validation procedure should be clearer. Please specify what “K” represents and how the spatial blocks were defined.

Response:

We have revised the description of the spatial cross-validation procedure in both Section 3.4 and Table 1. The revised text now explicitly states that K denotes the number of spatial folds, with K = 5 in this study. Samples were first grouped into fixed 5° × 5° latitude–longitude blocks according to their profile locations, and these blocks were then randomly assigned to five mutually non-overlapping spatial folds using a fixed random seed. In each fold, one complete spatial fold was withheld as the spatially independent test set, while 20% of the remaining non-test blocks were used for validation and the rest for training. Table 1 has been revised accordingly.

4. Comment:

Throughout the manuscript, the usage of “temperature-salinity” is inconsistent, with both en-dashes and hyphens appearing. Please standardize the notation.

Response:

We thank the reviewer for pointing this out. We have standardized the notation throughout the manuscript and now consistently use “temperature–salinity” with a dash when referring to combined temperature and salinity features or profiles. Other ordinary compound modifiers were kept with hyphens following standard usage.

We again thank the reviewer for the constructive comments. We believe that these revisions have substantially improved the transparency, methodological clarity, reliability assessment, and interpretability of the reconstructed 3D Chl-*a* dataset.

Reference

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