Detailed Responses

Here, we provide detailed responses to the referees’ comments. The comments from the referees are shown in black. Our responses to the critics of the referees are supplied in normal font and blue. The appropriate correction in the manuscript has been repeated in red font in the response letter.

Referee #2:

The manuscript and datasets submitted by Zhang et al. proposed a thorough scheme AIGD-PFT using deep learning techniques to retrieve seamlessly eight phytoplankton functional types (PFTs) chlorophyll a concentrations on the global scale. The AIGD-PFT is built based on an extensive global in situ pigment data set and CMEMS products including satellite ocean color, physical and biogeochemical data sets based on model simulations covering the year from 1998 to 2023. All CMEMS data were preprocessed to have the same spatial resolution. Before performing the deep learning ensemble for PFT retrievals, a gap-filling technique DCT-PLS was firstly applied to all the global CMEMS products to generate seamless data on the global scale. The STEE-DL model were trained and established based on ResNet models using Monte Carlo and bootstrapping methods to finally estimate the PFT chlorophyll a concentration with corresponding model uncertainty assessment. Products were intercompared with other PFT data based on different methods and model simulations and showed outstanding performance.

This work demonstrated thoroughly the seamless PFT products on the global scale over the last 26 years and has shown high potential of machine learning/deep learning techniques in ocean color applications, and here especially for PFT information retrievals. This study delivered the first gap-free global PFT products. I find it significant and the study has put a big step forward for the phytoplankton group estimation using multiple products based on big-data deep learning methods. However, I have several comments and suggestions (listed below) that the authors may consider to hopefully help improve further the quality of this work.

Response:

We are grateful for reviewing our manuscript and providing us with your
recognition and valuable advice on our work. Your comments and suggestions have helped us improve the manuscript.

Please check the item-by-item response, as well as the revised manuscript and supplementary materials. Note that the appropriate corrections in the manuscript have been repeated in red font in the response letter.

Abstract: ‘PFT values’ here indicate PFT chlorophyll a concentration, correct? This should be clarified in the beginning and kept consistent through the whole ms.

Response:

Thank you for your reminder. Yes, 'PFT values' here indicate PFT chlorophyll a concentration. We have revised it as follows (see Lines 17 on page 1 of the revised manuscript) and ensured consistency throughout the manuscript:

“The STEE-DL model utilizes an ensemble strategy with 100 ResNet models, applying Monte Carlo and bootstrapping methods to estimate optimal PFT chlorophyll a concentration and assess model uncertainty through ensemble means and standard deviations.”

L23-25 Have the time series and impact of climate change been reflected here? Otherwise it is not proper to put such statement here but can be more on a perspective tone.

Response:

Thank you for your comment.

In the paragraph (Lines 23-25) of the original manuscript, we aim to convey the potential applications of the AIGD-PFT product rather than present specific findings regarding the impacts of climate change. While the AIGD-PFT product provides comprehensive spatiotemporal data that aids in studying phytoplankton dynamics and their response to climate change, our current analysis does not directly quantify these impacts.

Based on your suggestion, we have removed the relevant statements.
Intro: L43: Put also reference for DPA, Vidussi et al. 2001

Response:

Thank you for your attention to detail. The reference has been correctly cited (see line 38-40 on page 2 of the revised manuscript).

“the separation of phytoplankton diagnostic pigments through High-Performance Liquid Chromatography (HPLC) with the assistance of Diagnostic pigment analysis (DPA, Vidussi et al. 2001) or CHEMTAX (Mackey et al., 1996) algorithms remains the most cost-effective and quality-controlled method to date (Swan et al., 2016).”


L54-55: I think there are a few more references in this regard, e.g.  El Hourany et al 2024, Li et al 2023 deep learning for pigments

Response:

Thank you. These references have been correctly cited (see line 50 on page 2 of the revised manuscript):

“…introducing more marine environmental covariates into ecological approaches (Zhang et al., 2023; Raitsos et al., 2008; El Hourany et al. 2024; Li et al. 2023) has become a current research focus…”


Sect 2.2.1 Indicate how many data were finally collected from all these sources

Response:

Thank you for your suggestion.

We have added Table S1 in the supplementary that details the number of data collected from each source:
Table S1 Reference and website for the publicly available in situ HPLC phytoplankton pigment dataset utilized in this study.

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L161 DINEOF – I think the original studies should be cited here too.

**Response:**

Thank you for your reminder. The reference has been correctly cited (see line 161 on page 9 of the revised manuscript).
“Previous studies have developed various methods for reconstructing missing pixels in remote sensing data, such as DINEOF (Data Interpolation Empirical Orthogonal Function) (Alvera-Azcárate et al., 2011; Liu and Wang, 2022),”


L 175 Normalisation: the dataset is standardized by dividing by the spatial mean, for each day or all 30 days together?

Response:

Thank you for your comments. In this study, the data normalization process is as follows: we first calculate the spatial mean for the entire dataset (from 1998 to 2023). Then, we standardize the data for each day by dividing it by this long-term mean.

The relevant text has been revised for clarity (see line 175 on page 10 of the revised manuscript):

“(2) Normalization: To minimize differences in dimensions and magnitudes of data across different spatial regions, the dataset is standardized by dividing by the spatial mean. The spatial mean is calculated from the entire dataset spanning from 1998 to 2023.”

L186-189: high missing values – not proper, high missing rates?

Response:

Apologies for the confusion.

The term “high missing values” should indeed be more accurately stated as “high missing rates”. We have corrected it (see line 190 on page 10 of the revised manuscript).

“It is important to note that in areas of high latitude with extremely high missing rates”

Seems that the authors have cut the data based on latitudes as there is a straight cutoff
in the maps?

Response:

Thank you for your comments.

We performed data cropping to minimize the common problems of missing data and low reliability at high latitudes. This method has been applied in previous research, and we have cited the relevant literature in our paper.

L195: Remove the ‘.’ or use comma after Table 2.

Response:

Thank you for your reminder. We have removed it.

L198-199: SSS – This CMEMS product contains data from 2019 to 2024 only. I suppose you used the physical analysis hindcast too. Should be both cited.

Response:

We apologize for the errors and confusion in our manuscript. We would like to clarify the specifics of the data used in our research as follows:

(1) **Sea Surface Temperature (SST) Data:** For SST, we utilized data from the ESA SST CCI and C3S reprocessed sea surface temperature analyses (DOI: [https://doi.org/10.48670/moi-00169](https://doi.org/10.48670/moi-00169)) which covers up to October 2022. For the period from November 2022 onwards, we employed the Global Ocean OSTIA Sea Surface Temperature and Sea Ice Analysis (DOI: [https://doi.org/10.48670/moi-00165](https://doi.org/10.48670/moi-00165)).

(2) **Sea Surface Salinity (SSS) Data:** We utilized the dataset Global Ocean Physics Reanalysis for SSS data (DOI: [https://doi.org/10.48670/moi-00021](https://doi.org/10.48670/moi-00021), Fig. #1-1). This dataset includes the subset cmems_mod_glo_phy_my_0.083deg_P1D-m covering data before June 2021, and the subset cmems_mod_glo_phy_myint_0.083deg_P1D-m covering from June 2021 onwards.

(3) **Biogeochemical Variables:** Regarding the biogeochemical variables, we used the Global Ocean Biogeochemistry Hindcast dataset (DOI: [https://doi.org/10.48670/moi-00019](https://doi.org/10.48670/moi-00019), Fig. #1-2), which consists of two subsets. Until December 2022, we used the subset cmems_mod_glo_bgc_my_0.25deg_P1D-m, and
from January 2023 onwards, we employed the subset cmems_mod_glo_bgc_myint_0.25deg_P1D-m.

We have added a clear statement (see line 198-207 on page 11 of revised manuscript), as follows:

“The SST data are sourced from the ESA SST CCI (Climate Change Initiative) and C3S (Copernicus Climate Change Service) global Sea Surface Temperature Reprocessed product (https://doi.org/10.48670/moi-00169, covering the period from January 1998 to October 2022) and Global Ocean OSTIA Sea Surface Temperature and Sea Ice Analysis (https://doi.org/10.48670/moi-00165, covering the period from November 2022 to December 2023). The SSS data are obtained from Global Ocean Physics Reanalysis (https://doi.org/10.48670/moi-00021). Biogeochemical data include nitrate concentration (NC), phosphate concentration (PC), silicate concentration (SC), and dissolved oxygen (DO). These variables are critical for understanding the nutrient dynamics in marine ecosystems, which are fundamental factors influencing phytoplankton growth and distribution. The data for these biogeochemical variables are sourced from the global biogeochemical multi-year hindcast products (https://doi.org/10.48670/moi-00019).”

L205: Resampling from lower resolution to high res might cause irreal data filling

Response:

Thank you for pointing out this important concern.

We agree with you. In our study, we opted to resample all physical and biogeochemical data to the same high 4 km resolution as the ESA-OC-CCI product primarily for consistency across datasets. We acknowledge that transforming data from a lower to a higher resolution often assumes that the newly generated pixel values are similar to the original ones, potentially introducing a so-called "false precision" that could lead to systematic biases.

To minimize the impact of false precision, the Inverse Distance Weighting (IDW) method was employed for spatial interpolation. The IDW identifies all available pixels around a target pixel based on a search radius of 8 pixels, and the weights of the identified available pixels are then calculated by the reciprocal of the square of the distance between the target pixel and the available pixels. This method is more likely
to provide balanced estimates and reduce the risk of introducing false precision.

With advancements in technology, the availability of high-resolution ocean data is increasing, such as *Multi-Scale Ultra High Resolution (MUR) Sea Surface Temperature data* (1km resolution, DOI: https://doi.org/10.5067/GHGMR-4FJ04), which provides hope for fundamentally addressing these issues. However, at present, offering datasets with varying spatial and temporal resolutions seems impractical. The resampling approach we have taken is a compromise intended to maximize the use of existing data resources while minimizing the computational and data processing burden. How to reduce information loss during data processing will be an important focus for our future work.

Follow your concerns, we have added a clear explanation about resampling (see line 207-212 on page 11 of revised manuscript):

“All data undergo the following preprocessing steps: (1) resampling, where all data is resampled to a 4km resolution using the pysample library (https://doi.org/10.5281/zenodo.3372769). The Inverse Distance Weighting (IDW) method was employed for spatial interpolation. The IDW identifies all available pixels around a target pixel based on a search radius of 8 pixels, and the weights of the identified available pixels are then calculated by the reciprocal of the square of the distance between the target pixel and the available pixels. This resampling process may lead to missing pixels, which are then filled using the nearest neighbor method;”

Additionally, the Discussion section has been expanded to include the following content (see line 523-528 on page 30-31 of revised manuscript):

“Firstly, in this study, all physical and biogeochemical data were resampled to match the high resolution of 4 km, consistent with the OC-CCI product, primarily to ensure uniformity across datasets, and to maximize the use of existing data resources. However, resampling from a lower to a higher resolution can indeed alter the statistical properties of the data, potentially introducing inaccuracies. In future research, it is planned to incorporate more high-resolution data and to minimize the loss of information during the data processing stage.”

Standardisation – is this step conflicting with the normalisation step 2 of the DCT-PLS?

Response:

Thank you for your comments. Although both standardization processes involve
data scaling and are technically similar, they serve two distinct purposes and operate independently within the processing workflow, with no conflict between them: (1) The normalization in DCT-PLS primarily aims at data reconstruction to ensure the completeness and continuity of the dataset; (2) The normalization used in the predictive model is designed to scale various input variables to a uniform level, thus enhancing the stability and effectiveness of model training.

L210-218: any basis/ references for these transformations?

**Response:**

Thank you for your comments. We have included relevant references in the revised manuscript to support the scientific basis for using these transformations (see line 216-217 on page 11 of revised manuscript):

“Incorporating spatial-temporal encoding into models is an effective strategy to enhance prediction accuracy, allowing for better capture of complex spatial-temporal interactions within the data (Yang et al., 2022; Wei et al., 2023).”


L225 Is the STEE-DL model different from that in Zhang et al. 2023? Why did not the authors use that approach but developed the current STEE-DL instead? Any advantages?

**Response:**

Thank you for your comments. We respond to the above two questions one by one as follows:

(1) Is the STEE-DL model different from that in Zhang et al. 2023?

Yes, the proposed STEE-DL model in this study is different from the model described in Zhang et al. 2023. The previous STEE model from Zhang et al. (2023) combines three different machine learning methods (Gradient Boosting Machine, 1D-
CNN, and TabNet) using ridge regression for ensemble learning. In contrast, the STEE-DL model is built around an ensemble of 100 ResNet models.

(2) Why did not the authors use that approach but developed the current STEE-DL instead? Any advantages?

In the previous research by Zhang et al. (2023), the focus was primarily on the generation of monthly PFT products, for which the STEE model was developed. The STEE model integrates three complex machine learning methods aimed at achieving high prediction accuracy. However, when the present study shifted from monthly to daily predictions, the computational demand increased significantly, turning the processing speed of the model into a critical bottleneck. Additionally, although the previous STEE model is capable of making high-precision predictions, it does not provide an uncertainty assessment for these predictions, which is a drawback in many ecological applications.

These challenges prompted the development of the STEE-DL model. The proposed STEE-DL model represents a significant improvement and expansion over the STEE model described in Zhang et al. (2023). It features major enhancements in the following two areas:

(1) **Running Speed**: The STEE-DL model is entirely based on a deep learning architecture and was specifically designed with computational efficiency in mind. By employing lightweight network designs and leveraging GPU acceleration, it significantly reduces the time required for computations. This enhancement is particularly important for our study's application scenario, which involves processing massive datasets to generate global, long-term daily PFT (Plant Functional Type) data series.

(2) **Uncertainty Assessment**: The STEE-DL model incorporates a deep learning ensemble framework, which not only improves prediction accuracy but also enables the direct assessment of prediction uncertainty—a capability not present in the Zhang et al., 2023 model. By calculating the ensemble mean and standard deviation of the model outputs, the STEE-DL provides a quantified range of uncertainty for each prediction. This feature is extremely valuable for scientific research and decision-making support.

To clarify and follow your concerns, we have added a statement (see lines 229-236 on pages 12-13 of revised manuscript) as follows:

“In the previous research by Zhang et al. (2023), the focus was primarily on the generation of monthly PFT products, for which the STEE (Spatial-Temporal-Ecological Ensemble) model was developed. The STEE model integrates three complex machine learning methods aimed at achieving high prediction accuracy. However, when the present study shifted from monthly to daily predictions, the computational demand increased significantly, turning the processing speed of the model into a critical bottleneck. Additionally, although the previous STEE model is capable of making high-precision predictions, it does not provide an uncertainty assessment for these predictions, which is a drawback in many ecological applications. To address these challenges, the present study further developed the STEE-DL (Spatial–Temporal–Ecological Ensemble model based on deep learning).”

L232-233: reads strange. Rephrase the sentence - This setup decreases the dimensionality of features from 19 to 16, and then to 10, before a final fully connected layer maps these features to an output value for predicting the target variable.

Response:

We have rephrased the description to more clearly explain the model’s process from input to output and the changes in network dimensions (see line 245-247 on page 13 of revised manuscript):

“In this model, the input layer receives 19 feature variables, which are then reduced to 16 after the first residual block. Subsequently, the second residual block further reduces the number of features to 10. Finally, a fully connected layer maps these features to an output value for predicting the target variable.”

L245- put example references for statistical methods

Response:

Thank you for your suggestion. The relevant literature has been correctly cited as follows (see line 255 on pages 13 of revised manuscript):

“The variability among ensemble model outputs, quantified by the standard deviation ($\sigma$) of the 100 independent models, provides a measure of uncertainty in
predictions (Chau et al., 2022).”


L253: Does this show how the matchups between the in situ data and CMEMS products were extracted? I would indicate the number of the data points too - also later in the stats

Response:

Thank you for your comments. In this study, the matchup data were generated based on temporal and spatial proximities. Specifically, we used a temporal window of one day and a spatial window of four kilometers for the matchups.

We have included Figure S1 in the supplementary material to illustrate the number of data points (see line 272 on pages 14 of revised manuscript):

“Figure S1 in the Supplementary material presents the histograms of the Chl-a concentrations of the eight PFTs at log-10 scale.”

Figure S1 Log-scale histogram of Chl-a concentrations for eight PFTs and the number of in situ data points.

L288-L292: put this together this paragraph with the above one, or using bullets to describe the three CV procedures more clearly.
Thank you for your constructive feedback. Based on your suggestion, we have combined the mentioned sections and provided a clear description of the three cross-validation (CV) procedures. The revised section is as follows (see lines 293-309 on pages 15 of revised manuscript):

“Cross validation (CV) is a commonly used method for analyzing model performance, allowing for a comprehensive assessment of a model's accuracy, stability, and generalization. This study implements three types of CV methods: random five-fold CV, time-block five-fold CV, and spatial-block five-fold CV, to deeply evaluate the model’s multifaceted performance. Specifically, the methods are as follows:

1. Standard five-fold cross-validation: This method randomly divides all data into five equal-sized subsets. In each round of validation, one subset is selected as the test set, while the remaining four subsets serve as the training set, ensuring that each data point is used as test data. This method primarily evaluates the model’s performance and generalization on the entire dataset.

2. Time-block five-fold cross-validation: Data is divided into five consecutive time periods in chronological order. In each iteration, data from one time period is chosen as the test set, with the data from the remaining periods serving as the training set (as shown in Figure 5). This method takes into account the continuity and dependency of time series, helping to evaluate the model’s ability to capture time trends and seasonal variations.

3. Spatial-block five-fold cross-validation: Similar to time-block cross-validation, but data is divided based on spatial location. A hexagonal grid was created at 20° horizontal and vertical intervals, and regions without sampling points were removed for hexagonal regions. In each round, data from one geographical block is left out as the test set, while data from other blocks are used for training (as shown in Figure 6). This method prevents potential data leakage due to spatial autocorrelation and helps to assess the model's spatial prediction capability and its generalization across different geographical locations.”

L386: not sure if it is appropriate to call them ecological types.

Response:
Thank you for your comments. We have replaced “ecological types” by “functional types” in the revised manuscript (see line 404 on pages 23 of revised manuscript), as follows:

“Firstly, the model achieved high prediction accuracy for key functional types such as Diatoms, Dinoflagellates, and Green algae, with significant advantages at certain sites: for instance, at sites 4 and 5, the prediction correlation coefficients for Diatoms were as high as 0.90 and 0.88, respectively.”

L402-404: High missing rates in high latitudes limit the application there. Can the authors indicate the range of the latitudes for these seamless PFT products?

Response:

Thank you for your comments. Our PFT products are primarily applicable within the range of 75°S to 75°N. We have added a clear statement to indicate this range (see line 190 on pages 10 of revised manuscript), as follows:

“It is important to note that in areas of high latitude (above 75°) with extremely high missing values (exceeding 80%), these data will be directly removed (as demonstrated in the video example available at https://doi.org/10.5446/67366), because reconstruction under such conditions is impractical.”

22) Fig 12: Though it is demonstrated in the video, maybe yearly mean maps here can better demonstrate the whole global ocean - a daily product cannot cover both polar regions.

Response:

Thank you for your suggestion. We have included yearly mean maps in the supplementary material of the revised manuscript (see line 432 on pages 25 of revised manuscript), as follows:

“Additionally, the yearly mean maps for 2020 are provided in Figure S2 of the supplementary, showing the distribution pattern of global ocean PFT throughout the year.”
Figure S2 The yearly mean global distribution of Chl-a concentration in 2020 for (a) Diatoms, (b) Dinoflagellates, (c) Haptophytes, (d) Pelagophytes, (e) Cryptophytes, (f) Green Algae, (g) Prokaryotes and (h) Prochlorococcus. The grey areas represent lands.

Fig 13 and uncertainty: I see all data were log transformed, how were these uncertainties calculated in the original conc.?

Response:

We apologize for the mistake in Figure 13. Indeed, all computations of the
uncertainties in this study were conducted on logarithmically transformed data, which follows conventional practice in the field of ocean color research.

We have corrected Figure 13 and added a detailed explanation (see line 258 on pages 13 of revised manuscript), as follows:

“It should be noted that all computations of the uncertainties in this study were conducted on logarithmically transformed data, which follows conventional practice in the field of ocean color research (Xi et al., 2021).”


Figure 13 The global distribution (2020-03-10) of the uncertainties for (a) Diatoms, (b) Dinoflagellates, (c) Haptophytes, (d) Green Algae, (e) Prochlorococcus, (f) Prokaryotes, (g) Pelagophytes and (h) Cryptophytes.

L504-505: From Fig 13 the model uncertainties one can see already large uncertainties for certain PFT in some regions, such as diatoms and cryptophytes with very low chla values (<0.01 mg m-3) in the gyres but with uncertainty larger than 0.1 mg m-3 and also for Prochlorococcus in high latitudes (almost not existing) with very high uncertainty.
Response:

Thank you for your comments. We apologize once again for the unit error in Figure 13 and would like to clarify that the uncertainties were actually calculated on a logarithmic scale, not in mg m\(^{-3}\), as previously corrected.

Regarding the high uncertainties in regions with low chlorophyll concentrations that you mentioned, there are two main reasons: (1) Insufficient training data. The lack of sufficient training data to represent these extreme conditions limits the model's ability to generalize the distribution of PFT in these areas, resulting in increased predictive uncertainty. (2) Intrinsic detection limits of the model. At very low chlorophyll concentrations, the sensitivity and accuracy of remote sensing technology can decrease, leading to a significant increase in relative uncertainty of predictions.

In future research, we are committed to improving the model's performance under these extreme conditions by incorporating more diverse and representative data.

L512 Discussion: How easy is it to apply the STEE-DL model to future datasets? I find it might be difficult to apply it as one has to prepare and preprocess all input data and fill the gaps using the DCT-PLS. That might be an obstacle to put it into operational. The authors should discuss on this point too.

Response:

Thank you for your reminder.

The STEE-DL model requires a relatively complex data preprocessing, including data cleaning, normalization, and filling gaps using the DCT-PLS method. Although these steps increase the workload before deploying the model, they are essential to ensure the quality and integrity of the model input data.

To reduce the complexity of these steps, we are developing more user-friendly data preprocessing tools, which will help users prepare data more easily.

Are the authors planning to publish the codes of AIGD-PFT in the future, so that the others can test it with their own prepared data sets?

Response:
Thank you for your comment. We plan to open source STEE-DL model and related tools in the future. This will include the complete data processing pipeline, model training, and prediction codes.