Algorithm Theoretical Basis Document For

Analysed Chlorophyll products

Sr	Product Name	Spatial	Temporal
No.		Resolution	Resolution
1	E06OCM_L4_AC	0.25° × 0.25°	Daily

1. Algorithm Configuration Information

- 1.1 Algorithm Name: Analysed chlorophyll fields for the global ocean using Particle Filter technique
- 1.2 Algorithm Identifier: E06OCM_L4_AC
- 1.3 Algorithm Specification

Version	Date	Description	Prepared by
1.0	16/12/2024	Analysed chlorophyll fields for global ocean using Particle Filter technique	Smitha Ratheesh

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2. INTRODUCTION: Satellite measurements of ocean colour allow synoptic coverage of ocean biological production on a global scale. Satellite derived chlorophyll measurements provide global distribution of phytoplankton CHL-a on high spatial and temporal scale. The accurate measurements of ocean chlorophyll concentration are very critical to understand the regional and global impact of climate change on marine ecosystem. Considering the contribution of chlorophyll-a measurements to the characterization of Earth's climate, World Meteorological Organization (WMO) has identified CHL-a as one of the Essential Climate Variable (ECV) under ocean category. However, the continuous availability of satellite based CHL-a is a major challenge due to the obstruction of the visible part of the e.m spectrum by clouds. Moreover, the observations from ocean colour near coastal region suffer from inaccurate atmospheric correction due to the optical complexity in the coastal waters.

Coupled physical-biogeochemical modelling provides a key insight into the interaction of elements in the physical and biogeochemical system of marine ecosystem. The coupled models, thus become an essential tool in the scientific community to elucidate the mechanism of physical and marine system and

predict its evolution in both space and time scale. It enhanced the scope to study the biogeochemical and ecological responses to physical forcing, which is a key component in the climate change science and environmental risk assessment.

2.1 Overview and Background: The synergistic use of satellite derived chlorophyll and model simulated chlorophyll is adapted in order to explore the advantages offered by both systems in the generation of analysed fields of chlorophyll. For this purpose, daily fields of model chlorophyll from a coupled physical-biogeochemical model are modified with respect to satellite derived chlorophyll data by statistically combining both fields of chlorophyll using Particle filter technique for the global ocean. Particle Filter is an ensemble based technique like ensemble Kalman filter (van Leeuwen, 2009). But unlike methods like EnKF, ensemble optimal interpolation (Evensen, 2003) etc, particle filter doesn't change the dynamical balance of the system and also does not consider the *apriori* assumption of the Gaussianity of the probability distribution function (PDF) of the system. This makes particle filter more suitable for non-linear systems like ocean dynamics. Recently the particle filter techniques have been successfully utilized in assimilation of chlorophyll data in a coupled bio-physical model (Ratheesh et al., 2016) and in the assimilation of highly non-linear coastal waves in a wave models (Bhowmick et al., 2019).

2.2 Objective

The main objective of this document is to provide step wise implementation of the algorithm, along with required inputs and desired outputs. This document will form the basis of operational implementation of the algorithm.

2.3 Input data sets

2.3.1 Satellite Data: Chlorophyll-a global product from OCM3 onboard OCEANSAT-3 is used in the algorithm to improve model simulations of chlorophyll. GAC products are available scene wise at 1 km resolution wise (https://bhoonidhi.nrsc.gov.in). More than 200 scenes are available daily for the entire globe. Therefore, a gridded field of OCM-3 chlorophyll-a is generated as an intermediate product for the global ocean at 4km resolution combining all the OCM-3 products available for the particular day.

2.3.2 Model Data: Chlorophyll from coupled physical-biogeochemical model (MOM5-TOPAZ) for the global ocean is used as the background chlorophyll field in the algorithm. This model is operationally running at SAC.

2.3.2.1 General description of the Ocean General Circulation Model

Ocean General circulation model used for the simulation of physical parameters of ocean is Modular Ocean Model, version 5 (MOM-5). It is a numerical representation of the ocean's hydrostatic primitive equations employing either Boussinesq (volume conserving) or non-Boussinesq (mass conserving) kinematics. The present study use Boussinesq kinematics. This model is developed by NOAA's Geophysical Fluid Dynamics Laboratory (GFDL) in Princeton, USA. The horizontal grids used in MOM5 are generalized horizontal coordinates, with the coordinates assumed to be locally orthogonal. For global ocean climate modeling, MOM uses the tripolar grid that has a bipolar Arctic region (Murray , 1996). The model also employs a split-explicit time stepping scheme where fast two-dimensional dynamics is sub-cycled within the slower three dimensional dynamics. MOM gives a wide array of vertical mixing schemes and the present model configuration used KPP scheme.

2.3.2.2. Description of the Ecosystem model

The present configuration for global ocean is a coupled one, in which MOM5, the ocean component is coupled to an ocean ecosystem model. A comprehensive model of oceanic ecosystems and biogeochemical cycles is used to understand and simulate the ocean ecosystem. The model used is Tracers Of Phytoplankton and Allometric Zooplankton (TOPAZ). TOPAZ is a state of the art model that considers 22 tracers including three phytoplankton groups, two forms of dissolved organic matter, heterotrophic biomass, and dissolved inorganic species for C, N, P, Si, Fe, CaCO3 and O2 cycling. The model includes such processes as gas exchange, atmospheric deposition, scavenging, N2 fixation and water column and sediment denitrification, and runoff of C, N, Fe, O2, alkalinity and lithogenic material. The phytoplankton functional groups undergo co-limitation by light, nitrogen, phosphorus and iron with flexible physiology. Loss of phytoplankton is parameterized through

the size-based relationship of Dunne et al. (2012b). Particle export is described through size and temperature based detritus formation and mineral protection during sinking with a mechanistic, solubility-based representation alkalinity addition from rivers, CaCO3 sedimentation and sediment preservation and dissolution.

For each model state variable C , the continuity equation is solved

$$\frac{\partial C}{\partial t} = -\nabla . \, \tilde{u}C + \nabla K \nabla c + S_C$$

Where \tilde{u} is the velocity vector from the OGCM, *K* is the diffusivity, and S_c is the sum of the sources and sinks for state variable C.

2.3.2.3 Coupled biogeochemical - physical model (MOM5-TOPAZ)

The coupled biogeochemical - physical model is configured for global ocean with a horizontal resolution of 25 km and a variable vertical resolution with a very fine near surface and coarser towards the bottom of ocean. There are 50 levels in the vertical direction. The external time step used is 22.5 sec and the internal time step used is 1800 sec. The model bottom topography is derived from the 2 minute resolution ETOPO 2 database. The surface salt is restored to climatology on a time scale of 2 months.

During spin up, the physical model was forced by climatological wind and flux data sets and was initialized with temperature and salinity data from Levitus. The model was spun up for 50 years from rest. Afterwards, TOPAZ model is coupled with the physical model and performed a climatology run for another 10 years. For this nitrate, phosphate and silicate are initialised using data from WOA13. After this, an inter-annual run is performed using the daily forcing fields of wind, net short and long wave radiation, precipitation, air temperature and specific humidity from NCMRWF from 2018 onwards. Model forecast is also performed using the NCMRWF data sets for the next 8 days. Model forecasts are written for every six hours, while the analysis fields are written daily.

2.3.3 Other Auxiliary data: None

Table 1: Input data sets for the algorithm

Data sets	Spatial Resolution	Temporal
		Resolution
Chlorophyll from	25 km x 25 km	Daily
coupled model		
Chlorophyll from	1 km	Daily
OCM-3 (GAC		
product)		

3. Algorithm Functional Specifications

In this section we describe the theoretical basis and algorithm overview for generating daily analysed fields of ocean surface chlorophyll for the global ocean.

3.1. Overview

OCM-3 derived chlorophyll products are assimilated into the coupled model using particle filter technique to generate more improved fields of model chlorophyll state. Bootstrap technique is used to generate particles/ensembles from model background field, which is chlorophyll field at ocean surface. A gridded field of OCM3 derived chlorophyll fields at 4 km is generated daily for the global ocean as an intermediate product. These three major steps in the algorithm are shown in Figure 1.



Figure 1: Major steps involved in the generation of analysed chlorophyll product

3.2. Generation of 4km gridded fields of OCM-3 derived Chlorophyll (Intermediate product): GAC products of chlorophyll for the global ocean are available scene wise and includes many number of GAC data products for a single day. Therefore, an intermediate product of OCM-3 chlorophyll is generated daily for the global ocean at

4 km resolution. For the purpose, firstly a background data with 4 km pixel resolution is generated for the global ocean. Secondly, each of the GAC products are scanned location wise and corresponding chlorophyll value is allotted to the specific 4 km pixel corresponding to the location. Figure 2 shows flowchart of generating the gridded fields of OCM-3 chlorophyll for the global ocean. For an example, the gridded OCM-3 derived chlorophyll for the global ocean is shown for 28 November 2023. More than 200 GAC scenes were considered to generate gridded OCM-3 product for the mentioned day.



Figure 2: Flowchart of gridded 4 km OCM-3 chlorophyll data for the global ocean.



Figure 3: Gridded 4 km OCM-3 derived Chlorophyll for the global ocean for 28 November 2023. Some of the GAP scenes for the same day are also shown. More than 200 GAC scenes were considered to generate gridded product for a day.

3.3. Theoretical Background of Particle Filter technique

The algorithm used for the assimilation of satellite derived CHL into the coupled model is a state of the art ensemble based particle filter technique. Particle filtering

uses a set of particles to represent the posterior distribution of a stochastic process given noisy and/or partial observations. The novelty of the scheme lies in the fact that, unlike other ensemble technique, particle filter does not impose any restriction on the form of the PDF of the background field. Thus, its superiority in nonlinear and non-Gaussian systems makes it widely acceptable to many applications (van Leeuwen, 2009, 2010). The realistic implementation of Particle filter is explained in Mattern et al., 2013; Ratheesh et al., 2016 and Bhowmick et al 2019.

Particle filtering method approximate the posterior distribution using randomly extracted particle sets from the posterior probability. The central concept is to determine the distribution of the system's state variable with minimal variability or uncertainty, and is achieved by updating the probability distribution of the state variable based on observed data and system dynamics. The cornerstone of particle filter is Bayes's theorem which reads

$$p_m(\psi|d) = \frac{p_d(d|\psi)p_m(\psi)}{p_d(d)} \tag{1}$$

Where:

- *p_m(ψ|d)* is the Posterior distribution, representing the true state of the system generated using model simulated chlorophyll (ψ) given chlorophyll observations (*d*) from OCM-3.
- 2. $p_d(d|\psi)$ is the likelihood function, representing the probability of observing *d* given the prior information about the state of the system, which is the model simulated chlorophyll. This term plays a crucial role in assigning weights to the model particles based on their consistency with the observed data.
- 3. $p_m(\psi)$ is the prior information about the ocean surface chlorophyll, also known as background fields. These are obtained from coupled model simulations of chlorophyll. A set of randomly selected model particles represent the Probability Distribution Function (PDF) of the background fields.

The model PDF can be written as

$$p(\psi) = \frac{1}{N} \sum_{i=1}^{N} \delta(\psi - \psi_i)$$
⁽²⁾

where, N is the number of particles. ψ_i is spanning the range from 1 to N. The term $\delta(\psi - \psi_i)$ represents the PDF of an individual particle centered around its value ψ_i , where δ is the Dirac delta function. The number of particles in the study N is 250.

4. $p_d(d)$ is the probability of observations. Its computation can be challenging, particularly in scenarios with sparse observations. This probability is not directly computed but is implicitly represented by the sum of weights of particles (w_i). These weights, assigned to each particle based on its likelihood of matching the observations, collectively form a probability distribution. Normalizing the weights ensures that they sum up to one, effectively representing the likelihood of observing *d* across all particles. Thus, the $p_d(d)$ can be written as:

$$p_d(d) = \sum_{i=1}^N w_i \tag{3}$$

where w_i is the weight of each particle computed with respect to the observations.

The computation of weights is a crucial step in the particle filter technique and is represented by:

$$w_i = \frac{p(d|\psi_i)}{\sum_{i=1}^N p(d|\psi_i)} \tag{4}$$

Therefore, w_i represents the likelihood of observing d given each particle ψ_i compared to the total likelihood of observing d across all particles. As mentioned earlier, weights are already normalized so that their sum is unity. Weight is inversely proportional to the distance between a given observation and its model background. The distance is taken to be usual root mean square difference between model chlorophyll and OCM-3 derived chlorophyll, taken over those model grids where observations are available on a particular day. Thus, the particles close to observation receive more weight as compared to farther ones. In this study, model particles of chlorophyll close

to OCM-3 derived chlorophyll assign large weightage and becomes strong particles, while weak particles are discarded. The posterior distribution is then represented by the set of particles with stronger weights. These particles, with higher weights, are considered to be more likely to represent the true state of the system based on the available observations.

3.4. Particle filter and its implementation procedure

One critical aspect of the ensemble-based approach in high-dimensional coupled models is the generation of a large number of ensembles or particles needed to closely approximate the posterior probability density of the system. Particle generation in this study is done using bootstrapping sampling by introducing random biases to the background field (Bhowmick et al 2019). This approach substantially reduces the computational time required for particle generation, which otherwise needs a distinct model run for each particle generation in the conventional particle filter techniques. The random Gaussian biases are computed with zero mean and 0.5 mg/m3 standard deviation. Here, we used standard deviation of the model chlorophyll to define the PDF of random biases. The randomly introduced biases are then modified for each model grid point with respect to both the model chlorophyll values at each grid point and the model bias. In this way, the correction term added to the model chlorophyll varies spatially with respect to the values of chlorophyll at that grid location. Model bias is computed from the long-term model simulations with respect to satellite-derived chlorophyll and its value is 0.3 mg/m3. This method results in a total of 250 particles being drawn by introducing biases to the background field.

Another important step in the Particle Filter technique is the selection of strong particles to represent Posterior PDF. This is done using a sequential importance resampling (SIR) method (van Leeuwen 2009, Bhowmick et al., 2019, Bhowmick et. al. 2023) to ensure robust estimation of the posterior distribution. The basic idea is to discard particles with low weights and retain multiple copies of particles with relatively higher weights, keeping the total number of particles the same. Selection of particles based on its weight is

carried out using Sequential Importance Resampling (SIR) method. In this method, weights are first normalised ([0 1)] and then added to form a cumulative distribution. A random generator is used to generate random numbers and the weights close to this random number is selected from cumulative distribution and this process is repeated multiple times. Probability is very high for choosing particles with higher weight from a cumulative distribution. Thus, the weights for each particle are computed, and the particles are resampled, assigning them equal weights (1/N). N is the total number of ensembles generated. This weight calculation and resampling process is how observations are assimilated into the model. Particle degeneracy is a common problem associated with ensemble-based techniques, where a very few particles carry significant weights, while the majority have negligible weights. This leads to a loss of diversity in the particle population and inaccurate representation of the posterior distribution. SIR addresses this issue by retaining the multiple copies of stronger particles and ensuring that the particle population remains diverse during the resampling process, where particles are randomly selected based on their weights. Assigning equal weights to all selected particles during resampling ensures that each particle has an equal chance of being selected. This prevents the loss of valuable information and improves the sampling efficiency and robustness of the sampling variability.

The flowchart of generating analysed chlorophyll fields for the global ocean is given in Figure 4.



Figure 4 : Flow chart of the methodology for generating analysed chlorophyll fields

3.5. **Operational Implementation:** The implementation steps that are to be followed are mentioned below and is also shown in Figure 5.

Step 1: Daily fields of ocean surface chlorophyll output generated from MOM5-TOPAZ coupled model in MOSDAC is considered as the model background data.

Step 2: OCM-3 GAC chlorophyll data downloaded from Bhunidhi NRSC site is considered as the observation.

Step 3: Checking the availability of model and OCM-3 data. If both data sets are available, following steps (steps 4 - 6) will be carried out to generate final product of analysed chlorophyll field.

Step 4: Generation of daily gridded fields of OCM-3 Chlorophyll combining all GAC products for the particular day.

Step 5: Preparation of 250 ensembles from model background field using Bootstrap technique.

Step 6: Generation of daily analysed fields of chlorophyll for the global ocean using Particle Filter technique.



Figure 5: Steps involved in the Operational Implementation

3.6 Output: Daily fields of chlorophyll from coupled model is improved using particle filter technique incorporating OCM-3 derived chlorophyll data. Therefore, the output generated is available at the same temporal and spatial resolution of the coupled model, which is at 25 km spatial resolution and daily.

3.6.1. Format of Output : The outputs are available as images (jpeg format) and product file (nc format). The analysed chlorophyll fields displayed in the Gallery section in the MOSDAC is shown in Figure 6 for the day 25 January 2024.





3.7 Initial Validation

For inter-comparison and validation, independent observations of satellite and Bio-Argo buoys are used for the period September 2023 to November 2023.

3.7.1 Analysis with Multi-Satellite Chlorophyll data

For validating the analysed products, results are compared with available satellite observations. For the purpose, we have used chlorophyll data from sensors other than OCM-3 such as MODIS, VIIRS, etc. This validation can be considered as an independent validation as these satellite information is not incorporated while generating the analysed chlorophyll product. A merged product of chlorophyll from these satellites are downloaded from https://marine.copernicus.eu.

To generate analysed chlorophyll fields, OCM-3 derived chlorophyll is assimilated to the coupled model simulated chlorophyll to improve the model simulations of surface chlorophyll. Therefore, validation is carried to check the improvement brought to the model simulations through the incorporation of OCM-3 data. Figure 7 shows the weekly average of chlorophyll (15 Oct 2023 to 22 Oct 2023) from various sources; 1) Coupled model chlorophyll, 2) Analysed Chlorophyll, 3) Chlorophyll from OCM-3, and 4) Merged Chlorophyll data from multi-satellites. It is clear from Figure 7 that analysed chlorophyll fields capture the chlorophyll features in the ocean as observed in the multi satellite data. However, a slight overestimation is observed in the analysed products towards polar region beyond 60° latitude in both the hemispheres and is partially attributed to the sparse observations of OCM-3 in those regions and the bootstrapping sampling used in the study. While sampling, all the model points are altered adding random biases to the background filed. These particles are then compared with OCM-3 chlorophyll data to select strong particles as mentioned in the methodology section. Therefore, quantity and quality of OCM-3 observations play crucial role in the generation of more accurate analysed fields of chlorophyll. OCM-3 shows a positive bias all over the ocean with respect to multi-satellite chlorophyll data.



Figure 7: Chlorophyll from various sources averaged over the period 15 Oct to 22 Oct 2023. a) Coupled model chlorophyll, (b) Analysed Chlorophyll, c) OCM-3 derived Chlorophyll, and d) Merged product from multi satellites.

Figures 8 and 9 show mean and standard deviation of chlorophyll from different sources. It is very vivid from the figures that assimilation of OCM-3 data improved model simulations of chlorophyll. Analysed fields of chlorophyll is more close to chlorophyll observations from multi-satellite as compared to model simulations of chlorophyll and OCM-3 derived chlorophyll. The features of wind-driven upwelling induced chlorophyll concentrations in the western Arabian are enhanced in the analysed chlorophyll fields due to OCM-3 integration compared to chlorophyll simulations from coupled model without OCM-3 data.



Figure 8: Mean of the ocean surface chlorophyll: a) Coupled model chlorophyll, b) Analysed Chlorophyll, c) OCM-3 derived Chlorophyll, and d) Chlorophyll from multi satellites.



Figure 9: Standard deviation of the ocean surface chlorophyll: a) Coupled model chlorophyll, b) Analysed Chlorophyll, c) OCM-3 derived Chlorophyll, and d) Chlorophyll from multi satellites

3.7.2 Comparison with Bio-Argo data

Independent validation of the analysed chlorophyll and merged chlorophyll from multi-satellites has been conducted using Bio-Argo measurements. Bio-Argo is an extension of the Argo program, incorporating biogeochemical observations, including chlorophyll-a concentration, oxygen concentration, pH, and more. These floats are deployed and managed by an international community in coordination with institutes from various countries (Wong et al., 2020). Bio-Argo floats are downloaded from https://biogeochmical-argo.org.

Figure 10 shows the buoy locations used for the comparison. Multi-satellites chlorophyll, Analysed Chlorophyll, and model simulated chlorophyll without OCM-3 are compared with buoy measured chlorophyll and the statics are shown in the Table 1. Percentage error is computed using the equation $\frac{RMSE \text{ of } CHL}{Bio-Argo Mean CHL} * 100.$

RMSE is found less for the analysed chlorophyll compared to multi-satellite derived chlorophyll when compared against Bio-Argo data. One added

advantage in the Analysed chlorophyll is the availability of data at all ocean points. Another reason is that collocated points are less in the case of multisatellite data and is owing to the data void due to cloud obstruction. This issue does not affect analysed chlorophyll data as it is generated by combining chlorophyll observation with model simulation, providing chlorophyll at all model grid points. Additionally, analysed chlorophyll has the advantage of model simulations and observations and it's the errors are less compared to other two individual components such as model simulations and observations. Analysed chlorophyll OCF data exhibits a positive bias of 0.24 mg/m³ and is partially attributed to the positive bias in OCM-3 chlorophyll observations. Among the three CHL datasets, analysed CHL shows a lower percentage error, indicating better performance.



Figure 10. Bio-Argo buoy locations for the validation period.

Table 1 : Statistics obtained	l against BIOARGO data
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	Model	Analysed	Multi-
	Simulated	CHL (With	satellite
	CHL	OCM-3)	CHL
	(without		
	OCM-3)		
Collocated points	7843	7843	3502

Bias (mg/m3)		0.485	0.24	-0.16
RMSE (mg/m3)		0.6508	0.53	0.97
Correlation Coefficient		0.46	0.43	0.57
Percentage	error	100.49	81.84	149.78
$\left(\frac{RMSE \ of \ CHL}{Bio-Argo \ Mean \ CHL} * 100\right)$				

3.8 Generation of Analysed Chlorophyll fields using latest version of OCM-3 data

The latest version of the OCM-3 product available at NRSC Bhoonidhi site is used to generate analysed chlorophyll products as suggested by the ATBD review committee. Chlorophyll from various sources for the days 02 Jan 2025 and 10Jan2025 is shown in figures 11 and 12.



Figure 11: Chlorophyll from various sources for the day 02 Jan 2025. a) Coupled model chlorophyll, (b) Analysed Chlorophyll, c) OCM-3 derived Chlorophyll (New Version), and d) Merged product from multi satellites.



Figure 12: Chlorophyll from various sources for the day 10 Jan 2025. a) Coupled model chlorophyll, (b) Analysed Chlorophyll, c) OCM-3 derived Chlorophyll (New Version), and d) Merged product from multi satellites.

3.9 Results from CA (SPPU, Pune) under Oceansat-3 project

The analysed chlorophyll products have been used by Savitribai Phule Pune University (SPPU), Pune, CA under Oceansat-3 project. As suggested by the ATBD review committee, a part of their work with analysed chlorophyll fields are also included here. Monthly analysed chlorophyll for the global ocean has been generated by SAC at 25 km resolution using multi-satellite derived chlorophyll and TOPAZ model for the duration 1998 to 2015 and is provided to CA for their study. Seasonally varying compensation depth have been computed for the Indian Ocean using the OTTM (Ocean Tracer Transport Model) model and analyzed Chlorophyll-a provided by SAC and is shown in Figure 13.

Compensation depth is then used for computing export production for the Indian Ocean.



Figure 13: Seasonal mean of varying compensation depth (1998-2015) using analysed chlorophyll data from SAC

4.0 Limitations: The algorithm, as mentioned depends on the quality of the chlorophyll data simulation, observation (OCM-3 derived chlorophyll) and the sampling method adopted for generating multiple ensembles. Additionally, the model is not currently forward-integrated with the improved initial conditions of chlorophyll.

4.1 Future Aspect: The algorithm used here is to generate analysed ocean surface chlorophyll. A fully fledged data assimilation scheme, which sequentially incorporates the modified model fields into the model future projections is planned as future work. The possibility of assimilating Bio-Argo measured chlorophyll and the use of the optimal Interpolation technique to generate analysed chlorophyll fields for the global ocean will also be explored.

4.2 Potential Users of the data: One of the highlight of the analysed CHL products is the gap-free data for the global ocean. This analysed CHL products are beneficial for studies related to biogeochemistry, PFZ, carbon export, time series analysis, distribution of

chlorophyll in the ocean, interaction of eddies and chlorophyll, etc. Some of the expected end-users of this product are INCOIS, SSPU, NIO, etc

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