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NECCTON

NEW COPERNICUS CAPABILITY FOR TROPHIC OCEAN NETWORKS

Deliverable D5.1

Technical specification of the pelagic lower trophic level products

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Preface

This document is the deliverable D5.1 of the Task 5.1 of NECCTON. Its objective is to define the products and services for the pelagic lower trophic level component of the ocean ecosystem. It has been co-developed by Work Package (WP) 5 and the project stakeholders.

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Glossary

Product	In NECCTON, a "product" is the output of a model, or of a coupled model, developed in the project. The product is assessed as a potential new variable for the Copernicus Marine Service. Each product can be delivered as a number of co-products, e.g., by different models in different regions. Each co-product is composed of a set of sub-variables and delivered as a model-output dataset.
Sub-variable	In NECCTON, a sub-variable is a single component of the product that is simulated by the model and used to estimate the desired product. For example, suspended particular matter is a product that may be estimated as the sum of sub-variables representing matter with different sizes.
Dataset	The NECCTON products will be delivered in the form of "datasets". These are aggregations of model outputs or observations, having the same geospatial structure or feature type (e.g., profiles, point-series, trajectories, points, grid-series, grids). A dataset contains data relative to one or more products developed by NECCTON. It is composed of one or several data files. The aggregation is done so that the content of the dataset is FAIR for the user (findable, accessible, interoperable, and reusable) and expandable when the product is updated (time axis).
Datacube	The NECCTON "datacube exploratory viewer" is an interactive application for exploring and visualizing the datasets, adapted to the visualization of the NECCTON products simulated by the integrated ecosystem model. This datacube is based on innovative cloud-based technologies and will use a serverless architecture that allows it to connect directly to files and not to a server. This viewer will guarantee high-availability, visual analysis, and flexible data dissemination to the users
Service	In NECCTON, a service is a tool (e.g., software) that transforms the data of a product into information needed by a stakeholder for a specific application. Most notably, the NECCTON datacube is a service that will map features of the data selected by the user.
Derived product	In NECCTON, a derived product is the output of a service, which is calculated from an original product and other relevant information, in response to user needs. For example, the space-time occurrence of suspended particulate matter above chosen thresholds is a derived product, that could be an output of the NECCTON datacube.

Publishable Summary

The NECCTON D5.1 report provides a clear definition of the pelagic lower trophic level products that will be delivered by WP5 in the future development of NECCTON. It is intended to serve as a reference for internal and external users of the products. The definitions are based on the requirements of users that emerged from the NECCTON workshop "Co-design of future products" which was held on-line in June 2023 (more than 100 stakeholders attending) and the online survey "Product co-design" which was live from July to September 2023 (more than 200 respondents). In this document, the definition of the products includes a brief review of previous and ongoing efforts in defining and delivering the product in an operational framework, as well as a description of the expected exploitation by users and associated impact.

This document also describes the model datasets produced by NECCTON to deliver the products to internal and external users. These descriptions include a reference to the model producing the dataset, as well as features of the model output datasets, such as: their spatial coverage and resolution, and their temporal extension and resolution. It also includes a description of the metadata provided in the files containing the datasets. The observations expected to be compared to the model data are also listed.

The models that will be developed by NECCTON WP 5, as well as the accuracy and precision of the products, will be assessed using observations and quantitative metrics – consistent with the Copernicus Marine Service validation protocols – and will be the object of future deliverables.

WP 5 will deliver an ambitious 20 new model products with all the existing CMEMS modelled regions delivering at least one new product. The new products include Mesozooplankton biomass, Micronekton biomass, Suspended Particulate Matter, Particulate Organic Matter, Dissolved Organic Matter, and Reflectance. The new products are expected to benefit work on carbon budgeting and higher-trophic-level modelling in particular.

The engagement of stakeholders to tailor the WP 5 NECCTON products to user needs will continue throughout the duration of the project through the co-design of thirteen case studies, dedicated workshops and the engagement of other European projects, initiatives and networks (including the Copernicus Marine Service user groups).

1. Introduction

1.1 Scope of document

The objective of this document is to provide a clear definition of the pelagic lower trophic level products that will be delivered by NECCTON WP 5, and to serve as a reference for internal and external users of the products. The definition is based on the requirements of users that emerged from the NECCTON workshop "Co-design of future products" which was held on-line in June 2023 (more than 100 stakeholders attending) and the survey "Product co-design" held from July to September 2023

(more than 200 respondents). In this document, the definition of the products includes a brief review of previous and ongoing efforts in defining and delivering the product in an operational framework, as well as a description of the expected exploitation by users and associated impact.

This document also describes the model datasets that will be produced by NECCTON to deliver the product to internal and external users. These descriptions include a reference to the model producing the dataset, as well as features of the data, such as: their spatial coverage and resolution, and their temporal extension and resolution. It also includes a description of the metadata provided in the files containing the datasets. We also list the observations expected to be used to either calibrate the models or assess as the accuracy and precision of the products, using quantitative metrics, consistent with the Copernicus Marine Service validation protocols.

All the products and datasets delivered by NECCTON follow the FAIR principles: they are findable, accessible, interoperable and reusable (see the "Data Management Plan" D1.1). They will be disseminated using the NECCTON Datacube, which adheres to the FAIR principles. Their compatibility with the datacube is also described here.

A full description of the models used to produce the new pelagic lower trophic level products and datasets in WP 5, the datacube itself, and all derived products and the product quality/uncertainty, is deferred to later NECCTON deliverables, including "D5.2 – Report on integrated pelagic model developments".

For reference, the terminology used here, as defined in the glossary, has been adapted from that used in the Specification Sheets of the Essential Ocean Variables, defined by the Expert Panels of the Global Ocean Observing System (GOOS). GOOS is an Intergovernmental Oceanographic Commission (IOC)-led programme (https://www.goosocean.org). Whenever available, we used the Climate and Forecast (CF) standard metadata conventions or criteria to define the metadata of the NECCTON products and sub-variables (e.g., long-names, units; https://cfconventions.org/). When these were not available, we made here new propositions, following the CF criteria, that might be refined through the engagement of experts and users during the future delivery of the project, by using this document as a discussion platform.

1.2 Intended audience and reference to user needs

This document is designed as a guide for the NECCTON partners as well as future users of the new products delivered by WP 5 of NECCTON. WP 5 is working closely with WP 1 (Management), WP 2 (Stakeholders) and WP 9 (Case studies) to ensure these products correspond to user needs.

The user needs for the WP 5 products emerged from the session "WP 5 New and Improved Capabilities for pelagic lower trophic level modelling" of the NECCTON workshop "Co-design of future products" held on-line in June 2023 (more than 30 stakeholders attending the specific session) and the WP 5 dedicated section of the survey "Product co-design", held from July to September 2023 (more than 200 respondents).

An analysis of the attendants and results of the above workshop session and survey section indicated that most of the respondents identified as scientists or researchers (79 % for the online survey; 86 % for the workshop). In the online survey, 64 % of the respondents worked in academia, with the remainder working for other organisations, including non-governmental organisations and consultancies. In the online survey, which had the most respondents (n=224), all the products to be delivered by WP 5 were requested by at least one third of the survey participants. The most popular product was Dissolved Organic Matter (DOM), which was requested by 63 % of respondents. Feedback, expected use and impact for each single product, based on the analysis of the results, is provided in Section 3.

The engagement of the stakeholders to tailor the WP 5 NECCTON products to the user needs will continue throughout the duration of the project through the co-design of thirteen case studies, dedicated workshops and the engagement of other European projects (e.g., EU Horizon EcoScope, MARCO-BOLO, SEAMLESS, EDITO), initiatives and networks (including the Copernicus Marine Service user groups).

1.3 Structure of the document

The document is structured as follows. Section 2 provides a synthetic list of the products that will be delivered by WP 5. Section 3 provides a thorough description of each product, including: i) a general definition; ii) the user requirements, iii) the current state of the art, iv) planned evolution of the product delivery, v) the observations expected to be used to assess the model datasets, vi) the expected exploitation and impact of the product, and vii) key metadata of the product. Section 4 describes the datasets planned in NECCTON to deliver the products to users. A summary of possible challenges and expected impacts is given in Section 5.

2. Products summary

The NECCTON products (see definition in the glossary) that are delivered by WP 5 are listed in Table 2.1, along with selected, high-level information. This provides the reader and product users with an overview of the data delivered by NECCTON. The products are produced by marine ecological and biogeochemical models. In general, different models have been developed for the different regions. The models include PISCES (Aumont et al. 2015) which is used in the Global domain; SEAPODYM (Lehodey, Senina, and Murtugudde 2008) which is used for the Iberia-Biscay-Irish domain; ERSEM (Butenschön et al. 2016) which is used in the Northwest Shelf domain; ECOSMO II (Yumruktepe, Samuelsen, and Daewel 2022) which is used in the Arctic domain; ERGOM (Neumann, Siegel, and Gerth 2015) which is used in the Baltic domain; BAMHBI (Grégoire, Raick, and Soetaert 2008) which is used in the Black Sea domain; and the BFM (Salon et al. 2019) which is used in the Mediterranean Sea domain.

The product and dataset specifications can be accessed in Sections 3 and 4. The datasets are delivered by non-assimilative hindcasts (H), i.e. model simulation of the past, or observational (O) datasets in

the special case of PRISMA hyperspectral data. These are named with unique numeric identifiers (H1, H2, ….) and (O1, O2, …) respectively.

Table 2.1 List of the co-products delivered by WP 7. First column: name of the product; second column: product ID; third column: ID dataset used to support the development of the product; fourth column: Copernicus Marine Service region; fifth column: model to be used for creating the product; and sixth column: NECCTON partner responsible for delivering the product.

Name product	ID co.product	ID datasets	Region	Partners
Mesozooplankton biomass	1.1	H4	Arctic	NERSC
Mesozooplankton biomass	1.2	H2	North-West (NW) European Shelf	UKMO
Mesozooplankton biomass	1.3	H5	Baltic	BSH
Mesozooplankton biomass	1.4	H1	Global	Moi
Mesozooplankton biomass	1.5	H36	Iberia-Biscay-Ireland	CLS
Micronekton biomass	2.1	H15	Global	CLS
Micronekton biomass	2.2	H36	Iberia-Biscay-Ireland	CLS
Suspended Particulate Matter	3.1	H2	NW European Shelf	UKMO
Suspended Particulate Matter	3.2	H3	Black Sea	UoL
Particulate Organic Matter	4.1	H4	Arctic	NERSC
Particulate Organic Matter	4.2	H6	Mediterranean Sea	OGS
Particulate Organic Matter	4.3	H2	NW European Shelf	UKMO
Particulate Organic Matter	4.4	H5	Baltic	BSH
Dissolved Organic Matter	5.1	H4	Arctic	NERSC
Dissolved Organic Matter	5.2	H2	NW European Shelf	UKMO
Dissolved Organic Matter	5.3	H5	Baltic	BSH
Reflectance	6.1	O1	NW European Shelf	CNR
Reflectance	6.2	O2	Black Sea	CNR
Reflectance	6.3	O3	Mediterranean Sea	CNR

Reflectance	6.4	H6	Mediterranean Sea	OGS
Reflectance	6.5	H5	Baltic	BSH
Reflectance	6.6	H3	Black Sea	UoL
Reflectance	6.7	H2	NW European Shelf	UKMO

3. Product definition

The next sections provide thorough definitions of each distinct product listed in Table 2.1.

3.1 Product Mesozooplankton biomass

3.1.0 Introduction

Mesozooplankton are heterotrophic organisms in the size range from 0.2 to 20 mm. Mesozooplankton move with ocean currents but can migrate vertically in the water column. Mesozooplankton generally feed on primary producers, microzooplankton and detritus particles. They are an important prey for fish larva and planktivorous fish and therefore represent an important link between primary producers and higher trophic levels.

3.1.1 User feedback and requirements

There was good interest in the mesozooplankton product from the stakeholders with >80 out of 184 respondents from the online survey being interested in obtaining a mesozooplankton biomass product. For the survey performed during the NECCTON Stakeholder workshop, the participation was lower (21-22 respondents per question). Here, about 40 % of the respondents were interested in mesozooplankton biomass. All respondents wanted the variable to include an uncertainty metric. Among the various geographical domains about 50 % of the respondents were interested in mesozooplankton biomass in the Arctic and Iberian-Biscay-Irish domain while more than 70 % were interested in mesozooplankton on the Northwest Shelf and in the global domain. In the Baltic about 40 % of respondents were interested in the product. Most respondents wanted the output on a grid with a spatial resolution of a few kilometres or less, and a depth resolved product was preferred to a depth-averaged one. Daily frequency was the preferred temporal resolution, followed by monthly frequency.

3.1.2 State-of-the-art on product delivery and gaps

Currently no operational service (to our knowledge) delivers mesozooplankton biomass as a product. There is currently a total zooplankton biomass product provided for the global, the Arctic, the Baltic, the Ibereia-Biscay-Irish and Mediterranean Sea regional domains in the Copernicus Marine Service. The reason has been that mesozooplankton is often the closure variable in biogeochemical models, and the associated mortality from predation is poorly parameterised. Furthermore, there are a limited number of datasets available for validating mesozooplankton biomass as predicted by models. Thus, this variable has been considered to have a high uncertainty. Mesozooplankton is an output from

earth system models participating in the Carbon Model Intercomparison Project (CMIP) 6, but only 5 of the participating models provide this variable.

3.1.3 How NECCTON will innovate the product and fill the gap

In NECCTON, we will first improve the representation of mesozooplankton in biogeochemical models by improving the representation of two key processes: vertical migration and mortality. Zooplankton are preyed upon by both tactile and visual predators, with visual predators better able to find their prey when there is light. Vertical migration occurs on a daily cycle, with mesozooplankton staying at depth during the daytime to hide from visual predators. They then ascend to the surface at night to feed. In addition to affecting the mortality of zooplankton, this process also influences carbon export in the ocean (Steinberg and Landry 2017). Including vertical migration will change the depth of mesozooplankton feeding, defecation and mortality. Additionally, we will implement a light-dependent mortality parameterization for mesozooplankton to represent the reduced efficiency of visual predators in low light conditions. Based on these improvements, NECCTON will deliver depth-resolved mesozooplankton biomass in five regions: the Global Ocean, Iberia-Biscay-Ireland (IBI), Baltic, Arctic, and Northwest Shelf domains. The mesozooplankton product for the IBI domain stands alone in the sense it will be delivered along with the micronekton product using the SEAPODYM model coupled to PISCES.

3.1.4 Observational data needs for product calibration/assimilation/validation

For model validation we will use the mesozooplankton datasets from COPEPOD (https://www.st.nmfs.noaa.gov/copepod/about/databases.html) that provide observations on zooplankton abundance as well as a gridded ¼° climatology. We will also compare the model results to a 1° climatology of mesozooplankton (O'Brien and Moriarty 2012). For initial calibration of diel vertical migration, an acoustic dataset will be used (Cannaby and Ingvaldsen 2023). There will be no assimilation of this variable.

3.1.5 Expected users' uptake

We expect that mesozooplankton biomass will be of interest to modelers of higher trophic levels. We also expect that long timeseries of mesozooplankton biomass will be of interest to assessing ecosystem change in various regions of the ocean.

3.1.6 List of co-products, sub-variables and metadata in the data-files for this product

Co-product ID	**Co-product**
1.1,1.2 ,1.3,1.4,1.5	**Mesozooplankton biomass**
Sub-variable name [unit]	***Mesozooplankton carbon*** [mmol m^{-3}] *
Description	Carbon concentration from mesozooplankton (0.2 – 20 mm) component alone *
Long name	Mesozooplankton concentration in units of carbon *
Short name	zmeso *
Standard_name	mole_concentration_of_mesozooplankton_expressed_as_carbon_in_sea_water *
* available CF metadata (https://cfconventions.org/) If not starred, the metadata is newly proposed in NECCTON	

3.2 Product Micronekton

3.2.0 Introduction

Micronekton is a group of marine organisms characterized by a size range from 2 to 20 cm. It gathers various taxa and encompasses crustaceans, fish, and cephalopods. It constitutes an intermediate compartment of the oceanic trophic web as it feeds on zooplankton and it is the main prey of larger marine predators. Micronekton is considered to be a key player in the biological pump. It performs diurnal vertical migration (DVM) based on predation pressure. These organisms migrate every day between the surface where they feed during the night, and the deep ocean where they hide from predators during the day.

3.2.1 User feedback and requirements

There is a significant interest in the micronekton product; 30 % of the respondents to the online survey use the existing CMEMS product, and around 35 % users are interested in new developments or improvements. The spatial resolution required for users' activities is mostly a few kms (> 35 %, followed by 'Below 1 km': 25 %), and 3D in space (60 %). For the temporal resolution, more than 50 % of the respondents are interested in a daily product, and 25 % in a monthly product.

3.2.2 State-of-the-art on product delivery and gaps

The product *Global Ocean low and mid trophic levels biomass content hindcast* provided (DOI: 10.48670/moi-00020) by CMEMS is a 2D field of biomass content of zooplankton and six functional groups of micronekton distinguished according to their migration depth. It uses the LMTL component of the SEAPODYM dynamical population model (http://www.seapodym.eu). The product covers the Global Ocean with a spatial resolution of 0.083° × 0.083°, and a daily temporal resolution from 1998 to 2021.

The existing model SEAPODYM LMTL is forced by net primary production, euphotic depth, depth of each pelagic layer that zooplankton and micronekton inhabit, average temperature and currents over the pelagic layers. No data assimilation has been done. This model doesn't consider the two-way interactions between micronekton and biogeochemical cycles. As micronekton is a key player in the biological pump, studying biogeochemical fluxes in lower trophic levels can be a breakthrough in micronekton modelling.

3.2.3 How NECCTON will innovate the product and fill the gap

The study carried out as part of NECCTON focuses on micronekton modeling in its environment, by coupling the numerical model of micronekton population dynamics SEAPODYM-LMTL and the biogeochemical model PISCES, which represents carbon fluxes in the lower trophic levels. It will be carried out using the FABM framework in one dimension, thus modeling a simple water column. Then the 1D coupled model will be applied in homogeneous mesopelagic provinces, covering the Global Ocean and the IBI domain. This way, we will provide a Global Ocean and regional micronekton product, that considers biogeochemical fluxes in low and mid trophic levels. The final product will be delivered on a 2D spatial grid in each case, which accounts for dynamic variations in the size of biogeographical provinces.

3.2.4 Observational data available for product calibration/assimilation/validation

The observational data used for product validation and calibration are mostly acoustic data. A global database of 477 acoustic transects acquired between 2004 and 2019 is available. The 38 kHz-acoustic backscatter database is a compilation of different databases listed below. IMOS BA-SOOP (Integrated Marine Observing System, Bio-Acoustic Ships of Opportunity sub-facility) is an Australian database maintained by the CSIRO (available through Open Access to Ocean Data (aodn.org.au)), where data are mainly situated in the South Indian Ocean and the South Pacific Ocean. BAS (British Antarctic Survey) is a database (bas.ac.uk) with data around South Georgia and between the UK and South Georgia. Transects from IRD-CNRS (personal communication) are also used and come from campaigns funded by the Mycto-3D-MAP project (Southeast Indian Ocean) and the PIRATA project (equatorial Atlantic Ocean). Data delivered by personal communication from Elliot Lee Hazen (Pacific Ocean), Nils Olav Handegard (MarEcho station in the Atlantic Ocean), and Reka Domokos (North Pacific Ocean) fulfil our dataset. There is no data assimilation in this study.

3.2.5 Expected users' uptake

This product is expected to be used to estimate the impact of micronekton on regional or global carbon budgets. It may also be of interest to higher trophic level models as a prey biomass estimation.

3.2.6 List of co-products, sub-variables and metadata in the data-files for this product

Co-product ID	**Co-product**
2.1,2.2	**Micronekton**
Sub-variable name [unit]	***Epipelagic Micronekton*** [g m^{-2}]
Description	Mass content of epipelagic micronekton expressed as wet weight
Long name	Mass content of epipelagic micronekton expressed as wet weight
Short name	mnkc_epi
Standard_name	mass_content_of_epipelagic_micronekton_expressed_as_wet_weight_in_sea_water
Sub-variable name [unit]	***Epipelagic Micronekton*** [g m^{-2}]
Description	Mass content of epipelagic micronekton
Long name	Mass content of epipelagic micronekton
Short name	mnkc_umeso
Standard_name	mass_content_of_epipelagic_micronekton_expressed_as_wet_weight_in_sea_water
Sub-variable name [unit]	***Migrant Upper Mesopelagic Micronekton*** [g m^{-2}]
Description	Mass content of migrant upper mesopelagic micronekton expressed as wet weight
Long name	Mass content of migrant upper mesopelagic micronekton expressed as wet weight
Short name	mnkc_mumeso
Standard_name	mass_content_of_migrant_upper_mesopelagic_micronekton_expressed_as_wet_weight_in_sea_water

Sub-variable name [unit]	***Lower Mesopelagic Micronekton*** [g m^{-2}]
Description	Mass content of lower mesopelagic micronekton expressed as wet weight
Long name	Mass content of lower mesopelagic micronekton expressed as wet weight
Short name	mnkc_lmeso
Standard_name	mass_content_of_lower_mesopelagic_micronekton_expressed_as_wet_weight_in_sea_water
Sub-variable name [unit]	***Migrant Lower Mesopelagic Micronekton*** [g m^{-2}]
Description	Mass content of migrant lower mesopelagic micronekton expressed as wet weight
Long name	Mass content of migrant lower mesopelagic micronekton expressed as wet weight
Short name	mnkc_mlmeso
Standard_name	mass_content_of_migrant_lower_mesopelagic_micronekton_expressed_as_wet_weight_in_sea_water
Sub-variable name [unit]	***Highly Migrant Lower Mesopelagic Micronekton*** [g m^{-2}]
Description	Mass content of highly migrant lower mesopelagic micronekton expressed as wet weight
Long name	Mass content of highly migrant lower mesopelagic micronekton expressed as wet weight
Short name	mnkc_hmlmeso
Standard_name	mass_content_of_highly_migrant_lower_mesopelagic_micronekton_expressed_as_wet_weigh t_in_sea_water

3.3 Product Suspended Particulate Matter

3.3.0 Introduction

Suspended particulate matter (SPM) is a collective term for the inorganic (e.g., mineral) and organic (e.g., detritus; see next section) particulates that are suspended in the water column. It is an indicator of sediment transport, water clarity and quality; and has important implications for pelagic and benthic productivity and erosion. It can also act as a vector for the transfers of pollutants and contaminants.

3.3.1 User feedback and requirements

More than half of the stakeholders who responded to the online survey indicated an interest in an SPM product with a clear preference for scales of a few kilometres and less at daily resolution or less, in applications that concern past reconstructions or short-term forecasts. The main interest in an SPM product is driven by applications that concern the implications of SPM for visibility, shading or as a vector for nutrient transport.

3.3.2 State-of-the-art on product delivery and gaps

Despite their importance, particularly in coastal waters, the organic and inorganic components of SPM are generally not part of operational marine modelling systems, including those of the Copernicus Marine Service.

3.3.3 How NECCTON will innovate the product and fill the gap

Based on existing parametrisations we will develop a flexible model component of inorganic suspended particulate matter for incorporation in physical-biogeochemical model systems that considers the horizontal and vertical transport of particles and the interaction with organic particles. Developments will be made in a highly resolved study area covering the Tyrrhenian Sea ensuring readiness of the parametrisation for the requirements of coastal applications. The project will deliver a single variable for inorganic SPM.

3.3.4 Observational data available for product calibration/assimilation/validation

CMCC hold data on SPM concentrations in the Tyrrhenian Sea which have been collected as part of a separate project. The data will be provided to the project in-kind and used along with existing in-situ datasets and remote sensing products for model calibration and validation. A combination of available SPM in-situ (e.g., from Station L4 in the Western English Channel) and remote sensing data will be used to evaluate model performance in the NWS and Black Sea domains.

3.3.5 Expected users' uptake

Based on the feedback from the stakeholder surveys, the main uptake of the SPM product should be in its exploration as a factor affecting water visibility and a driver of change in marine productivity via shading and nutrient provision.

3.3.6 List of co-products, sub-variables and metadata in the data-files for this product

Co-product ID	**Co-product**
3.1,3.2	**Suspended Particulate Matter**
Sub-variable name [unit]	***Inorganic suspended particulate matter*** [mg m^{-3}]
Description	Mass concentration of suspended inorganic matter in sea water
Long name	Mass concentration of suspended inorganic matter in sea water
Short name	spm_min
Standard_name	mass_concentration_of_inorganic_suspended_particulate_matter_in_sea_water

3.4 Product Particulate Organic Matter

3.4.0 Introduction

Particulate Organic Matter (POM) in the ocean is operationally defined as all combustible organic matter that can be retained on a filter (Kharbush et al. 2020). The filter mesh size is typically 0.7 µm. It is often discussed in terms of Particulate Organic Carbon (POC), which reflects the important role POC plays in the ocean carbon cycle. The definition explicitly excludes Particulate Inorganic Carbon (PIC). The finite mesh size means the contribution of organisms smaller than 0.7 µm – including most

photosynthetic and non-photosynthetic prokaryotes – is not captured in measurements. At the other end of the size spectrum, the contribution of large, motile zooplankton is also not measured. Such organisms are either intentionally removed through filtering, or through sampling techniques which are designed to exclude larger, swimming organisms.

The operational definition of POM and POC contrasts with the definition used in most marine ecosystem and biogeochemical models. In marine ecosystem models, POM tends to be exclusively made up of non-living detrital material, including faecal pellets, the bodies of dead organisms, or other aggregations of organic matter.

3.4.1 User feedback and requirements

In the online survey, approximately 50 % of respondents expressed an interest in having a POM product in the CMEMS catalogue. >70 % of respondents were interested in having depth resolved data, while >65 % requested the data be daily in frequency. In the Stakeholder workshop, 80 % of respondents expressed an interest in have a product for POC. There was much less interest (<20 %) in both particulate organic nitrogen (PON) and particulate organic phosphorus (POP). Users were generally interested in both the living and non-living fractions of POM as well as total POM (approx. 50 % of users each). Users were most interested in a POM product for the Northwest Shelf domain (approx. 50 % of respondents). Approximately 20 %, 30 % and 35 % of respondents were interested in a POM product for the Arctic, Mediterranean and Baltic domains respectively.

3.4.2 State-of-the-art on product delivery and gaps

While phytoplankton carbon is provided by CMEMS for most of the CMEMS domains, total POC is not provided. Zooplankton carbon is only available in selected regions. Many models simulate both living POM and detrital POM. Detrital POM can also be split into size fractions which have different sinking speeds and interactions within the ecosystem. In addition, the sinking flux of POC is currently provided for the CMEMS Arctic domain (DOI: 10.48670/moi-00003).

3.4.3 How NECCTON will innovate the product and fill the gap

NECCTON will provide depth resolved, daily products for total particulate organic matter and detrital organic matter expressed as carbon (Particulate Organic Carbon (POC)) for the Northwest shelf, Arctic, Baltic and Mediterranean regions. Total POC encompasses both living and detrital components of POC. It is designed to match *in situ* ship-board measurements as much as reasonably possible. The living POC will consist of the sum of phytoplankton and small zooplankton (e.g., nano heterotrophic plankton and microzooplankton) biomasses. It will exclude mesozooplankton biomass due to the likelihood of them being missed in *in situ* sampling due to their ability to swim, sampling technique or potentially screening using a 200 µm mesh during sample collection. Bacterial biomass will also not be included in POC estimates as these will typically go through a 0.7 µm filter. The detrital organic matter product matches model definitions of particulate matter. PON and POP will not be delivered based on the limited user interest and lack of validation data for these variables.

3.4.4 Observational data available for product calibration/assimilation/validation

We will use a combination of validation products including satellite data (Sathyendranath, Kong, and Jackson 2022); BGC Argo data (Dall'Olmo 2021; Bellacicco et al. 2019) and *in situ* data. The provided

product for POC has been designed to closely mimic matchups with *in situ* data which the satellite data was validated from. Validation using BGC Argo floats may require exclusion of large size POM from model estimates as this method typically excludes large POM particles (Galí et al. 2022).

3.4.5 Expected users' uptake

Users are expected to use POC products to estimate the carbon budget of the ocean and carbon sequestration. POC may also be of interest to higher trophic level modellers as it can act as a food source for fish. In addition, there is interest in the POC flux to the benthos as it will impact the benthic system and can be used as a food source for demersal fish (provided in WP 6).

3.4.6 List of co-products, sub-variables and metadata in the data-files for this product

Co-product ID	**Co-product**
4.1,4.2,4.3,4.4	**Particulate Organic Matter**
Sub-variable name [unit]	***Total Particulate Organic Carbon*** [mol C m^{-3}]
Description	Sum of living particulate organic matter from 0.7-200 µm in size (phytoplankton + zooplankton not defined as mesozooplankton) and detrital organic matter, comparable to insitu POC observations
Long name	Total particulate organic matter (living+detrital)
Short name	tpoc
Standard_name	mole_concentration_of_particulate_organic_matter_expressed_as_carbon_in_sea_water
Sub-variable name [unit]	***Detrital Particulate Organic Carbon*** [mol C m^{-3}] *
Description	Sum of detrital particulate organic carbon components *
Long name	Sum of detrital particulate organic carbon *
Short name	detoc *
Standard_name	mole_concentration_of_organic_detritus_expressed_as_carbon_in_sea_water *
* available CF metadata (https://cfconventions.org/) If not starred, the metadata is newly proposed in NECCTON	

3.5 Product Dissolved Organic Matter

3.5.0 Introduction

Dissolved Organic Matter (DOM) is dissolved matter originating from living matter that operationally is not retained by filtration. It can be produced *in situ* from phytoplankton, zooplankton and bacteria and can also be of terrestrial origin. It is further modified through bacterial utilisation. Dissolved organic carbon is often separated into different fractions based on decomposition timescales into labile, semi-labile, semi-refractory and refractory pools. Commonly the refractory pool is not included within models as its turnover time is on the order of 100-1000s of years.

3.5.1 User feedback and requirements

There is high interest in the delivery of a DOM product through CMEMS, with approximately 60 % of respondents to the online survey (n=184) interested in using it. Most respondents were interested in a product with spatial resolution of a few kms (>35 %) with depth dependant information (>60 % of respondents), and on daily timescales (~ 50 % of users). In the stakeholder workshop, users were generally only interested in dissolved organic carbon (DOC) products (>80 % of respondents) and not dissolved organic nitrogen (DON) or dissolved organic phosphorus (DOP). There is some interest in having a total DOC product which includes a refractory, non-modelled DOC component (~25%), and individual labilities of DOC (~30%). Approximately (20 - 40) % of respondents in the interactive Stakeholder Workshop were interested in a DOM product for the Arctic, Northwest Shelf and Baltic Sea domains.

3.5.2 State-of-the-art on product delivery and gaps

Currently no MFCs provide any DOM products, although DOM is a state variable within some models. Generally, models only predict DOC with DON and DOP only available in the labile fractions. Different labilities of DOC are often modelled which represent different degradation timescales.

3.5.3 How NECCTON will innovate the product and fill the gap

For the first time, within NECCTON we will deliver depth resolved, daily products on total DOC for the Northwest Shelf, Arctic and Baltic regions. The total DOC defined here does not include the refractory component of DOC (typically ~40 uM) to be consistent with the CMOR definition of DOC (https://clipc-services.ceda.ac.uk/dreq/mipVars.html). The refractory component will be added on to the total DOC when validating the product against observations.

3.5.4 Observational data available for product calibration/assimilation/validation

Observational data for DOC is limited and is generally in the form of bottle data. Data will be taken from the global compilation of DOC data (Hansell et al. 2021), individual manuscripts/cruises (e.g., (Painter et al. 2018)) and observing stations (e.g., Western Channel Observatory; https://www.westernchannelobservatory.org.uk/). New satellite DOC products are in development. At the current time, they are not publicly available but will be considered for model validation if they become available during the project.

3.5.5 Expected users' uptake

The inclusion of DOC as a product is expected to help with the calculation of carbon budgets for the marine system.

3.5.6 List of co-products, sub-variables and metadata in the data-files for this product

Co-product ID	**Co-product**
5.1,5.2,5.3	**Dissolved Organic Matter**
Sub-variable name [unit]	***Total dissolved organic carbon*** [mmol m^{-3}] *
Description	T Sum of dissolved carbon component concentrations explicitly represented (i.e. not ~40 uM refractory unless explicit) *
Long name	Total dissolved organic carbon *

Short name	dissoc *
Standard_name	mole_concentration_of_dissolved_organic_carbon_in_sea_water *
* available CF metadata (https://cfconventions.org/) If not starred, the metadata is newly proposed in NECCTON	

3.6 Product Reflectance

3.6.0 Introduction

Reflectance (RRS) is the ratio of the electromagnetic flux reflected by a surface to the total electromagnetic flux incident on the surface. Water reflectance, as a function of the wavelength of electromagnetic radiation, provides useful information about the different types of suspended and dissolved components of matter in the ocean. It is used to identify various spectral features through the analysis of their inherent optical properties (i.e., absorption and backscattering). RRS is used to derive chlorophyll using empirical algorithms.

3.6.1 User feedback and requirements

There is good interest in the delivery of the reflectance product (approx. 40% of respondents to the online survey were interested). Most stakeholders required a product with spatial resolution of few kms (>28 %) or below 1 km (18 %), on a daily timescale (~ 35 % of users), with multiple spectral bands like Sentinel 3 OLCI (50 %) or hyperspectral imaging (28 %). Approximately 60 % of respondents are interested in reflectance for model validation. Both coastal and open ocean waters are of interest to stakeholders, with a focus on several biogeochemical variables (i.e., chlorophyll, CDOM and water turbidity). Respondents in the Northwest Shelf and Mediterranean domains had indicated an interest in an improved reflectance product (30 % and 28 % of respondents respectively).

3.6.2 State-of-the-art on product delivery and gaps

Currently no MFCs provide any reflectance products, although other optical products such as light attenuation (Kd) are provided for some regions.

3.6.3 How NECCTON will innovate the product and fill the gap

A new model derived reflectance product will be available. Exploitation of hyperspectral data usage from PRISMA combined with models will be tested for the first time. In the selected sites the L2 PRISMA data will be provided as an extra data product and compared with the models.

3.6.4 Observational data available for product calibration/assimilation/validation

The remote sensing reflectance acquired by satellite sensors is a marine Copernicus product. Therefore, the multi sensor L3 products available for each region provide direct validation for the models in the selected sites. The available multiyear multi sensors L3 products provide reflectance at 412 nm, 443 nm, 490 nm, 510 nm, 555 nm, 670 nm for the Mediterranean and Black Sea regions; 412 nm, 443 nm, 490 nm, 510 nm, 560 nm, 665 nm for the Baltic Sea region; and 443 nm, 492 nm, 560 nm, 665 nm, 704 nm, 740 nm, 783 nm, 865 nm for the NWS region. Water reflectance derived from PRISMA will be validated and compared with *in situ* matchups acquired with autonomous radiometers installed on stationary platforms.

3.6.5 Expected users' uptake

The reflectance product will be used for biogeochemical model validation, data assimilation in biogeochemical models and machine learning applications.

3.6.6 List of co-products, sub-variables and metadata in the data-files for this product

Co-product ID	**Co-product**
6.4,6.5,6.6,6.7	**Reflectance**
Sub-variable name [unit]	***reflectance*** [sr^{-1}]
Description	Remote sensing reflectance
Long name	Remote sensing reflectance
Short name	rrs
Standard_name	surface_ratio_of_upwelling_radiance_emerging_from_sea_water_to _downwelling_radiative_flux_in_air
6.1, 6.2, 6.3	**Reflectance**
Sub-variable name [unit]	***PRISMA reflectance*** [sr^{-1}]
Description	PRISMA Remote sensing reflectance
Long name	PRISMA Remote sensing reflectance
Short name	prisma_rrs
Standard_name	surface_ratio_of_upwelling_radiance_emerging_from_sea_water_to _downwelling_radiative_flux_in_air

4. Datasets description

The products described in Section 3 will be delivered in the form of "datasets" (see the definition in the glossary). All the 8 model datasets containing the products developed by WP 5, along with the 3 satellite datasets produced by WP4, are described in the following sub-sections.

4.1 H4 – Arctic domain

ID dataset	H4
Products names (product IDs)	Mesozooplankton biomass (1.1), POM (4.1), DOM (5.1)
Name sub-variables	zmeso, tpoc, detoc, dissoc
Geographical coverage	Arctic
Horizontal resolution	12 km
Vertical resolution	20 vertical layers
Time period	1991-2020
Temporal resolution	Monthly
Data-file(s)	neccton_nersc_h004_mod_arctic_ltl_hind_12km_P1M_mf-yyyymm

Expected total, max size of datafile(s) (Gb)	480 Gb (120 Gb per variable/sub-variable)
Format	NetCDF
Partner producer and contact	NERSC, Annette Samuelsen, annette.samuelsen@nersc.no
Datasets used for calibration/validation/assimilation	COPEPOD database for zooplankton, MAREDAT mesozooplankton climatology. POC, DOC and organic matter export in situ data at the Long-Term Ecological Research observatory HAUSGARTEN in the Fram Strait (source: PANGAEA), TOC and DOC (Lauvset et al. 2022), POM satellite data (Sathyendranath, Kong, and Jackson 2022) and BGC-Argo data (Dall'Olmo 2021; Bellacicco et al. 2019).
Method	Coupled HYCOM-ECOSMO (Yumruktepe, Samuelsen, and Daewel 2022) forced by ERA5 meteo, CMEMS global model boundary, climatical river volume fluxes and nutrient loads.

4.2 H2 – Northwest Shelf domain

ID dataset	H2
Products names (product IDs)	Mesozooplankton biomass (1.2), suspended particulate matter SPM (3.1), particulate organic matter POM (4.3), dissolved organic matter DOM (5.2), reflectance (6.7)
Name sub-variables	zmeso, spm_min, tpoc, detoc,, dissoc, rrs
Geographical coverage	Northwest European Shelf; -19 to 10 E, 41 to 64 N
Horizontal resolution	7 km
Vertical resolution	Variable, 50 vertical levels
Time period	1991-2020
Temporal resolution	Daily
Data-file(s)	neccton-ukmo_h002_mod_nws_ltl_hind_7km_P1D-m_mf-yyyymm
Expected total, max size of datafile(s) (Gb)	800 GB for the new variables only.
Format	NetCDF
Partner producer and contact	UK Met Office Susan Kay
Datasets used for calibration/validation/assimilation	Mesozooplankton: global plankton dataset COPEPOD (https://www.st.nmfs.noaa.gov/copepod/about/databases.html); climatology of mesozoplankton (https://doi.org/10.1594/PANGAEA.785501). SPM: remote sensing product, in situ data if available (e.g., Western Channel Observatory). POM: POM satellite data (Sathyendranath, Kong, and Jackson 2022) and BGC-Argo data (Dall'Olmo 2021; Bellacicco et al. 2019) and *in situ* data. DOM: global compilation of DOC data (Hansell et al. 2021), individual manuscripts/cruises (Painter et al. 2018) and observing stations (Western Channel Observatory). Satellite data if available.

Method	NEMO-FABM-ERSEM model with benthic component (Butenschön et al. 2016), with surface, boundary and river inputs as for the CMEMS NWS reanalysis.

4.3 H36 – Iberia-Biscay-Irish domain

ID dataset	H36
Products names (product IDs)	Mesozooplankton biomass (1.5), Micronekton biomass (2.2)
Name sub-variables	mnkc_epi, mnkc_umeso, mnkc_mumeso, mnkc_lmeso mnkc_mlmeso, mnkc_hmlmeso, mnkc_hmlmeso, zooc
Geographical coverage	Iberia-Biscay-Irish domain
Horizontal resolution	1/36°
Vertical resolution	3 layers based on the euphotic depth
Time period	2020-12-01 to 2023-12-31
Temporal resolution	daily
Data-file(s)	neccton-cls_h036_mod_ibi_ltl_hind_0.028deg _P1D-m_mf-yyyymm
Expected total, max size of datafile(s) (Gb)	Less than 10Gb
Format	NetCDF
Partner producer and contact	CLS Anna Conchon and Olivier Titaud seapodym-contact@groupcls.com
Datasets used for calibration/validation/assimilation	Meesozooplankton : O'brien and Moriarty (2012) Micronekton : IMOS acoustic database CSIRO micronekton biomass database
Method	SEAPODYM-LMTL (Lehodey, Senina, and Murtugudde 2008), using NEMO driving data and offline forcing of ocean color satellite data.

4.4 H5 – Baltic Sea domain

ID dataset	H5
Products names (product IDs)	Mesozooplankton biomass (1.3), Particulate Organic Matter (4.4), Dissolved Organic Matter (5.3), Reflectance (6.5)
Name sub-variables	zmeso, tpoc, detoc, dissoc, rrs
Geographical coverage	Baltic Sea – Lat 53.01 °N to 65.89 °N, Lon 9.04°E to 30.21°E
Horizontal resolution	Lat: 0.017 deg, Lon: 0.028 deg (~1 nm)
Vertical resolution	56
Time period	2018-2020
Temporal resolution	Daily

Data-file(s)	neccton_bsh_h005_mod_bal_pel_hind_1nm_P1D-m_mf-yyyymm
Expected total, max size of datafile(s) (Gb)	60 GB
Format	NetCDF
Partner producer and contact	BSH: Anja Lindenthal (anja.lindenthal@bsh.de); Josefine Hahn (josefine.hahn@bsh.de)
Datasets used for calibration/validation/assimilation	ICES database for Mesozooplankton; Satellite data OCEANCOLOUR_BAL_BGC_L3_MY_009_133 for Reflectance; CMEMS in-situ TAC for DOM and POM if available
Method	Coupled NEMO4.2.1-ERGOM forced by ERA5 Meteorology.

4.5 H6 – Mediterranean Sea domain

ID dataset	H6
Products names (product IDs)	POM (4.2), Reflectance (6.4)
Name sub-variables	tpoc, detoc, rrs
Geographical coverage	Mediterranean Sea
Horizontal resolution	4.5 km
Vertical resolution	125 Z levels: 1.5 m at surface, 10 m at 200m, and 100m at 3000m
Time period	1999-2020
Temporal resolution	daily
Data-file(s)	Folder:neccton-ogs_h6_mod_med_pel_hind_4.2_km_P1D-m_yyyymm
Expected total, max size of datafile(s) (Gb)	450Gb
Format	NetCDF
Partner producer and contact	OGS: Paolo Lazzari (plazzari@ogs.it); Gianpiero Cossarini (gcossarini@ogs.it)
Datasets used for calibration/validation/assimilation	BGC-Argo floats, Ocean color (OCEANCOLOUR_MED_BGC_L3_MY_009_143)
Method	Coupled OGSTM-BFM-OASIM forced by NEMO ogcm, climatological river inputs.

4.6 H41 – Black Sea domain

ID dataset	H41
Products names (product IDs)	SPM (3.2), reflectance (6.6)
Name sub-variables	spm_min, rrs
Geographical coverage	Black Sea
Horizontal resolution	15 km
Vertical resolution	59 vertical levels

Time period	Hindcast: 1999-2023
Temporal resolution	daily
Data-file(s):	neccton-uol_h41_mod_blk_ben_hind_15km_P1D-m_sf_yyyymm
Expected total, max size of datafile(s) [Gb]:	100 Gb
Format	NetCDF
Partner producer and contact	Loïc Macé, loic.mace@uliege.be
Datasets used for calibration/validation/assimilation	CMEMS in situ TAC
Method	Coupled NEMO-BAMHBI forced by MAR atmospheric conditions, climatological river inputs, RADTRANS.

4.7 H1 – Global domain

ID dataset	H1
Products names (product IDs)	Mesozooplankton biomass (1.4)
Name sub-variables	zmeso
Geographical coverage	Global
Horizontal resolution	1/4°
Vertical resolution	75 levels
Time period	1993-2020
Temporal resolution	daily/monthly
Data-file(s)	neccton-moi_h001_mod_glo_ltl_hind_0.25deg _P1D-m_mf-yyyymm neccton-moi_h001_mod_glo_ltl_hind_0.25deg _P1M-m_mf-yyyymm
Expected total, max size of datafile(s) (Gb)	50-100 GB
Format	NetCDF
Partner producer and contact	MOi, Coralie Perruche
Datasets used for calibration/validation/assimilation	Mesozooplankton: global plankton dataset COPEPOD (https://www.st.nmfs.noaa.gov/copepod/about/databases.html); climatology of mesozooplankton (https://doi.org/10.1594/PANGAEA.785501).
Method	NEMO-PISCES model forced by ERA5 atmospheric reanalysis.

4.8 H15 – Global domain

ID dataset	H15
Products names (product IDs)	Micronekton biomass (2.1)

Name sub-variables	mnkc_epi, mnkc_umeso, mnkc_mumeso, mnkc_lmeso mnkc_mlmeso, mnkc_hmlmeso, mnkc_hmlmeso
Geographical coverage	Global
Horizontal resolution	1°
Vertical resolution	Each group is defined on the layer(s) inhabited, meaning no explicit vertical dimension.
Time period	1998-2019
Temporal resolution	Monthly/Yearly
Data-file(s)	neccton-cls_h015_mod_glo_ltl_hind_1deg _P1M-m_mf-yyyymm
Expected total, max size of datafile(s) (Gb)	2-5 GB
Format	NetCDF
Partner producer and contact	CLS; Sarah Albernhe seapodym-contact@groupcls.com
Datasets used for calibration/validation/assimilation	Acoustic data
Method	SEAPODYM 2-way coupling with PISCES

4.9 O1 – Northwest Shelf Domain

ID dataset	O1
Products names (product IDs)	PRISMA reflectance (6.1.)
Name sub-variables	prisma_rrs
Geographical coverage	Selected site [30km x 30km] in Northwest Shelf.
Horizontal resolution	30 m
Vertical resolution	NA
Time period	2019-2023
Temporal resolution	Variable
Data-file(s)	neccton_cnr_o01_PRISMA_nws_obs_30m_yyyymmdd
Expected total, max size of datafile(s) (Gb)	20 Gb
Format	NetCDF
Partner producer and contact	CNR federica.braga@ismar.cnr.it
Datasets used for calibration/validation/assimilation	in situ reflectance acquired with autonomous radiometers installed on stationary platforms
Method	Extraction of PRISMA data.

4.10 O2 – Black Sea

ID dataset	O1
Products names (product IDs)	PRISMA reflectance (6.2)
Name sub-variables	prisma_rrs

Geographical coverage	Selected site [30km x 30km] in Black Sea.
Horizontal resolution	30 m
Vertical resolution	NA
Time period	2019-2023
Temporal resolution	Variable
Data-file(s)	neccton_cnr_o02_PRISMA_blk_obs_30m_yyyymmdd
Expected total, max size of datafile(s) (Gb)	100 Gb
Format	NetCDF
Partner producer and contact	CNR federica.braga@ismar.cnr.it
Datasets used for calibration/validation/assimilation	AERONET-OC in situ reflectance acquired with autonomous radiometers installed on stationary platforms
Method	Extraction of PRISMA data.

4.11 O3 – Mediterranean Sea

ID dataset	O3
Products names (product IDs)	PRISMA reflectance (6.3)
Name sub-variables	prisma_rrs
Geographical coverage	Selected sites [30km x 30km] in Mediterranean Sea.
Horizontal resolution	30 m
Vertical resolution	NA
Time period	2019-2023
Temporal resolution	Variable
Data-file(s)	neccton_cnr_o03_PRISMA_med_obs_30m_yyyymmdd
Expected total, max size of datafile(s) (Gb)	250 Gb
Format	Netcdf
Partner producer and contact	CNR federica.braga@ismar.cnr.it
Datasets used for calibration/validation/assimilation	AERONET-OC and other in situ reflectance acquired with autonomous radiometers installed on stationary platforms
Method	Extraction of PRISMA data.

5. Concluding remarks

WP5 will deliver an ambitious total of 20 new model products with all the existing CMEMS modelled regions delivering at least one new product. Users' pull for the new products was evidenced in both the online and interactive stakeholder surveys. Some challenges associated with incorporating multiple new developments into existing models are expected; and extensive validation against available observations will be critical for assessing the impact of each new development. The new products are expected to benefit work on carbon budgeting and higher-trophic-level modelling in particular.

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