Potential new higher-level products for Copernicus water research

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List of Acronyms

ASV	Autonomous Surface water Vehicle
AUV	Autonomous Underwater Vehicle
CDOM	Coloured Dissolved Organic Matter
CGLMS	Copernicus Global Land Monitoring Service
DIC	Dissolved Inorganic Carbon
DOC	Dissolved Organic Matter
EO	Earth Observation
ESA	European Space Agency
GLEON	Global Lake Ecological Observatory Network
HFM	High Frequency Measurements
MSI	Multispectral Instrument
NASA	The National Aeronautics and Space Administration
OLCI	Ocean and Land Colour Instrument
pCO2	Partial pressure of Carbon Dioxide
PP	Phytoplankton Primary Production
S2	Sentinel-2
S3	Sentinel-3
TP	Total Phosphorus
UV	Ultraviolet
VIS	Visible
WP	Working Package

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Table of Contents

Water-ForCE is a CSA that has received funding form the European Union's Horizon 2020 research and innovation programme under Grant Agreement No 101004186.

Executive Summary

This report analyses the user needs and currently available technical capabilities of different *in situ* sampling sensors to provide new higher-level biogeochemical products that could potentially be measured by combining different *in situ* sensors and satellite earth observation data.

There are some water related parameters and products (e.g. phytoplankton primary production) which until last decades have required a considerable amount of funds, time or work force to be estimated or measured, but can nowadays be estimated using automated high-frequency measurements (HFM). Using available HFM or proxies from satellite earth observation measurements, some of those products could be worked out and eventually implemented for future Copernicus water related services.

Our analyses on the state-of-the-art *in situ* monitoring knowledge bring out the recommendations that waterbodies mass primary production, concentration of dissolved organic carbon, partial pressure of carbon dioxide and concentration of total phosphorus can be estimated or calculated (with satisfactory accuracy) using a variety of different *in situ* measurement techniques or/and combining some proxy parameters from HFM in aquatic systems. Suggestions are given on what possible changes should be considered to build up those products, and how both *in situ* and remote sensing communities would benefit the most from each other's monitoring efforts.

Additionally, this report is also an input for the Water-ForCE WP2 Task2.4 where those analysed new possible products for Copernicus water related services will be described and explained from the Remote Sensing point of view according to the existing knowledge from the scientific research publications.

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1. Introduction

1.1 Water-ForCE

The Horizon-2020 project Water-ForCE (Water scenarios For Copernicus Exploitation) will develop a Roadmap for Copernicus Inland Water Services.

The Roadmap will contain:

- Analysis of user communities' landscape
- Analysis on how Copernicus water-related services can support policy development and monitoring of their implementation
- Gap analysis of the Copernicus water-related service portfolio
- Identification of future potential higher-level biogeochemical products
- Technical requirements for future Copernicus sensors to improve the water-related service portfolio
- Proposal for organising *in situ* measurement networks to validate Copernicus remote sensing and modelling products and to provide complementary data not collected by remote sensing
- Proposal on how to define relationships between Core Services and Downstream services
- Scenarios of the most optimal delivery of water services to different user communities.

The Water-ForCE project is coordinated by the University of Tartu (Estonia) with 20 participating organisations from all over Europe. It connects experts in water quality and quantity, in policy, research, engineering and service sectors.

This report is part of Work Package 4 (WP4) "Aligning *in situ* and satellite Earth observation activities" which is trying to establish clear links between *in situ* and satellite

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observation networks to ensure that they can mutually benefit from data collection and sharing.

1.2 Purpose of the document

The Space call (LC-SPACE-24-EO-2020) identified a specific element that should be addressed in the frame of the project – “development of high-level biogeochemical products, beyond basic variables for water quality and food web modelling or analysis”. This report brings out new potential higher-level biogeochemical products which could be developed as the future possible Copernicus water related services.

1.3 Content of the report

The combination of different sensors and the integration of new capabilities inside current *in situ* monitoring systems (buoys, ASVs and AUVs), together with remote sensing data, will allow both the direct monitoring of crucial inland water quality parameters or provide the needed data to indirectly derive them, enabling the development of higher-level remote sensing biogeochemical products that may become an essential part of Copernicus services. Task 4.5 analysed the user needs and currently available technical capabilities of different *in situ* sampling sensors and proposed new higher-level biogeochemical products that can potentially be measured by combining different *in situ* sensors and satellite earth observation data.

1.4 Higher-level products

One of the elements needed to be addressed in the frame of the LC-SPACE-24-EO-2020 call: Copernicus evolution: Mission exploitation concept for WATER is to “development of higher-level biogeochemical products, beyond basic variables for water

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quality and food web modelling analysis". However, the term "higher level" has not been well described and its use to define some products remains unclear. Looking from the *in situ* perspectives we can interpret that higher level products could be, for example: using information of one or more water quality parameters to predict or assume others which are not so easy to measure; or use more than one *in situ* measurements to feed a model that combines several input parameters into a new product. Last one could be used also in the case of modelling the food webs of the water bodies. Those two possible options were also considered in case of the current report. While the call itself is about Copernicus' future, we will also concentrate on the parameters and products which could be possible to be filled with existing remote sensing knowledge and available data.

2. User requirements

Discussions between Water-ForCE expert groups and different users and user groups meetings and workshops inside of the Water-ForCE WP1-5 activities have led to the identification of the main needs for future potential higher-level products which were felt to be of broad potential interest to those working with lake and coastal waters monitoring. Overall, users needed quick and easy knowledge of natural waters in terms of chemical, physical and biological parameters (e.g. dissolved oxygen concentration, pH, chlorophyll *a* concentration, water turbidity, total nitrogen and total phosphorus concentrations as well as dissolved organic matter concentrations). Additionally, users need to assess the change over time in water bodies to fill the requirements of different EU directives (e.g. Water Framework Directive, Urban Waste Water Directive, Nitrates Directive) and country-based water laws. Further to the requirements of different laws and directives, the interviews also highlighted some other specific needs (see Water-ForCE Deliverable 1.4):

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- Water quality and water levels (quantity) not only in major lakes, but also in smaller reservoirs and rivers and at much finer scale (catchment scale).
- Inclusion of microbial, toxin, algal, metal, and plastic pollution indicators.
- Detection of dissolved organic matter.
- Chlorophyll-a concentration in lakes and inland waters in general.
- Monitoring of fast-growing water plants and algae.
- Frequent mapping of CDOM (coloured dissolved organic matter)/DOC (dissolved organic carbon) products to assist on drinking water quality monitoring.
- Monitoring service for drinking water quantity and quality. Parameters such as a) cyanobacterial harmful algal blooms, b) Frequency of algal bloom occurrence.
- Monitoring of water quality in lakes and reservoirs used as drinking water sources.
- Surface temperature in coastal and inland water.

Those needs and requirements are an essential part of lake management. Needed monitoring outputs can be used as a tool to assess the health of the lake and to understand the impacts of human activities as well as natural processes. In addition, monitoring is a base for making good watershed management decisions and for evaluating the effects of these decisions. The monitoring techniques range from tests that can be performed occasionally by those with little training to full-scale, professional analyses in a well-equipped laboratory.

Many of those required variables are still difficult to measure directly from water bodies and therefore may require additional knowledge and laboratory working skills, a lot of workforce and time and available funds. Therefore, hydrobiological monitoring typically has monthly, rarely weekly resolution of water chemical, physical and biological data series and only the linear changes between subsequent measurements could be assumed.

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3. Possible new higher-level products

New higher-level products can be combined using the measured parameters from regular *in situ* (including some laboratory analyses) or/and automated high-frequency monitoring.

This chapter describes potential new products and their specific applications, giving details of the background knowledge and data requirements in aquatic studies. The number of possible higher-level products is wider than discussed in the Report. For this report, we analysed the entire list of needed products shown in chapter 2 of the current report, considering the technical possibilities that can be met with currently available *in situ* sensors. Based on this knowledge, we focused only on those products that at least theoretically could be developed and have the potential to be replaced or extended with remote sensing products in near future.

3.1 Primary production

Over the last century, a variety of approaches have been developed and employed for measuring the rates of production and the consumption of organic material in aquatic ecosystems. These processes, known collectively as “lake metabolism,” are closely related to trophic state and influence food web structure, energy transfer, carbon cycling, and greenhouse gas emissions in aquatic systems.

The pioneering work on coastal plankton metabolism in the 1920s included measurements of changes in dissolved O_2 concentrations during incubations of small bottles in light and darkness to estimate rates of primary production and respiration, respectively (Gaarder and Gran 1927). In fact, of all the methods used to measure aquatic ecosystem metabolism, the popularity of using incubations of water in bottles and chambers has persisted over time (Staehr et al. 2012), with subsequent developments

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using ^{14}C additions or tracing changes in dissolved inorganic carbon (DIC = CO_2 + HCO_3^- + CO_3^{2-}). Similar incubations of sediment chambers have been used to measure benthic photosynthesis and respiration, and when these rates are combined with bottle incubations of the water, they provide estimates of integrated ecosystem metabolism (e.g., Barko et al. 1977; Kemp et al. 1997; Gazeau et al. 2005a).

Phytoplankton primary production (PP) represents the major synthesis of organic matter in aquatic systems giving start to the food chains and forming the basis of the ecological pyramid. The amount of primarily synthesised organic matter indicates the trophic state of a waterbody, while the efficiency of its subsequent transformation in food chains results in a higher or lower fish production, and in a poorer or better water quality, therefore the data on the PP enable to get better understanding of the food web relationships in aquatic ecosystems.

Because of changing light conditions, PP has a pronounced diel pattern. In order to acquire integrated results over longer time periods (days, months, years), many consecutive measurements of instantaneous photosynthesis rate should be carried out and integrated. In some studies (Joniak et al., 2003; Yoshida et al., 2003; Forget et al., 2007) the values of daily PP integrated over the photic zone were estimated from *in situ* incubations. However, it gives the reliable results only in clear waters, while in highly productive waters we cannot perform the incubation during a long time (e.g., from morning to evening) as due to respiration of photosynthetic products (Lancelot & Mathot, 1986) and release of extracellular products (Møller Jensen, 1985), part of the ^{14}C-label gets lost from the cells during long-term incubation.

Direct measurements of PP are very time consuming, complicated, and expensive, not to mention the restrictions on the handling of the radioactive C in the *in situ* environment. It was not until the development of the diel curve technique (Sargent and Austin 1949, 1954) on a coral reef that ecosystem metabolism measurements became readily available for aquatic ecosystem studies. The method has been used

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extensively over the past four decades in all aquatic systems (Smith & Marsh 1973; Cole and Fisher 1978; Kemp and Boynton 1980; Barnes 1983; Gattuso et al. 1993; D'Avanzo et al. 1996; Caffrey 2003; Staehr & Sand-Jensen 2007; Coloso et al. 2008; Laas et al. 2012; Solomon et al. 2013; Cremona et al. 2016; Olesky et al 2021). The diel open-water technique provided a powerful alternative to bottle and chamber incubations, as it avoided the container artefacts and error propagation associated with incubations. This method allows measurement of aquatic ecosystem metabolism as changes in water column concentrations of O_2 or DIC *in situ* associated with photosynthesis during daylight and respiration at night (Odum 1956; Kenney et al. 1988). Although the open-water diel O_2/DIC technique has not changed fundamentally since the late 1950s, it is only in the last few decades that advances and expansion of relatively inexpensive and robust *in situ* high frequency sensing technology (especially measuring dissolved O_2) have made the measurements of metabolism easily tractable with the open water methods. This has radically increased the range of temporal and spatial scales of observations (e.g. Van de Bogert et al. 2007; Coloso et al. 2008; Hanson et al. 2008; Staehr et al. 2010; Solomon et al. 2013; Idrizaj et al. 2016; Giling et al. 2017).

Another alternative to the bottle incubations methods is to use bio-optical modelling methods. Bio-optical modelling is especially important in turbid waters of high productivity where the abrupt light gradient may cause large errors when traditional field methods are applied. A simple bio-optical model developed by Arst et al. (2008), where the basic equation describes the PP (in mg C m^{-3} h^{-1}) as a function of photosynthetically absorbed radiation and quantum yield of carbon fixation. The developed automated models for rapid estimates of phytoplankton primary production are a useful tool for filling the gaps in the measured primary production data and potentially extending the data series over periods for which other biological and chemical data are available. This helps to give a realistic estimation of the annual and interannual variability of primary production to be used in further ecosystem analyses.

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The previous results have demonstrated the suitability of the Arst et al. (2008) model for detailed description of vertical and temporal variation of the PP in lakes (Kauer et al., 2009; 2013, Nõges et al., 2011). The remote sensed data is a tremendous addition to the perspective of the PP estimations in the inland waters (Kauer et al., 2015; Soomets et al., 2019; 2020).

3.2 Dissolved organic carbon (DOC) and partial pressure of carbon dioxide (pCO_2)

Knowing the carbon content of inland waters and the carbon exchange between inland waters, the land, and the atmosphere is important from many different points of view. First, the need to understand and predict climate change and its impacts requires a solid comprehension of the global carbon cycle (Toming et al., 2020). Lakes and coastal waters play a crucial role in the global carbon cycle and therefore contribute to climate regulation (Pan et al., 2014; Tranvik et al., 2009, 2018). Secondly, while not directly harmful to human health, dissolved organic carbon (DOC) can have negative effects on the cost and effectiveness of water treatment, increasing the consumption of water treatment chemicals and fouls membranes used for filtration (Sharp et al., 2005; Zularisam et al., 2006). Additionally, DOC reacts with chemical disinfectants like free chlorine leading to the development of potentially toxic by-products (Herzsprung et al., 2012; Ledesma et al., 2012). Consequently, appropriate carbon data from surface waters will improve our understanding of the global carbon cycle and are highly needed for effective water treatment.

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3.2.1 Dissolved organic carbon (DOC)

Understanding of the true role of inland waters in the global carbon cycle requires reliable estimations of dissolved organic carbon, as up to 95% of organic carbon in lakes is in the dissolved form (Wetzel, 2001). ISO standard specifies a method for the determination of DOC in water (ISO 20236:2018). Measurements are typically conducted in the lab using special analysers that oxidise organic carbon in the water sample to form carbon dioxide. A detector then detects the released carbon oxide. Unfortunately, these methods need expensive laboratory equipment with high reagent costs. As an alternative, low-maintenance high-frequency optical sensors for measuring DOC are also available. The site-specific calibration is needed to get accurate results with those sensors. Unfortunately, part of the DOC is optically inactive and cannot be mapped directly by optical sensors. Coloured dissolved organic matter (CDOM) absorbs light and there is typically a strong correlation between DOC and CDOM in humic lakes where both parameters are fluctuating synchronously (Erlandsson et al., 2012; Tranvik, 1990). Therefore, CDOM can be used as a proxy in mapping lake DOC content in humic lakes. In non-humic lakes where DOC and CDOM do not vary synchronously the situation is much more complicated and the CDOM might not be a suitable predictor for DOC (Toming et al., 2016b). Molot and Dillon (1997) stated that if optical parameters are used as proxies for all or some fraction of DOC, then the mathematical relationship between these parameters and the DOC fraction must be time-invariant (Molot & Dillon, 1997). Unfortunately, it is not always so since CDOM and DOC concentrations might vary seasonally (Toming et al., 2016b). Therefore, it is difficult to find a proxy for describing the seasonal cycle of DOC in all lake types. Chlorophyll a, and total suspended matter or water transparency-related variables have been applied as proxies for DOC in eutrophic lakes (Toming et al., 2016b). Nevertheless, in large-scale interannual assessment, CDOM

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has been shown to be a powerful predictor of DOC and can also be applied for remote sensing of large-scale patterns of DOC (Toming et al., 2016b).

3.2.2 Partial pressure of carbon dioxide (pCO_2)

Carbon dioxide (CO2) is a key substance involved in a number of biogeochemical processes in natural waters (Atamanchuk et al., 2014). Inland waters are often supersaturated with aqueous carbon dioxide with respect to atmospheric CO2 and therefore, are broadly considered substantial sources of CO_2 to the atmosphere (Duarte et al., 2008; Kortelainen et al., 2006; Lazzarino et al., 2009; Raymond et al., 2013; Sobek et al., 2005; Tranvik et al., 2009; Laas et al. 2016). The most common parameter, which describes the amount of dissolved CO2 gas in water, is the partial pressure or pCO2 (Atamanchuk et al., 2014).

$$pCO2=P*x(CO2)$$

where x(CO2) = molar concentration of CO2 gas in the dissolved gas mixture (usually air) and P = total pressure of the gas mixture (Atamanchuk et al., 2014). Recent studies have revealed the presence of four interrelated processes closely associated with water surface pCO2, i.e., biological activities, physical mixing, a thermodynamic process, and the air-water gas exchange (Wen et al., 2021). Environmental and biogeochemical variables that can be linked with these processes are water surface temperature, water salinity, phytoplankton concentration, CDOM, latitude, mixed layer depth, etc. (Wen et al., 2021). The temporal and spatial distributions of pCO_2 in inland waters often exhibited high heterogeneity depending mostly on pH, water temperature (Kosten et al., 2010; Marotta et al., 2009; Pinho et al., 2016; Sobek et al., 2005), solar radiation (Yang et al., 2022), and trophic state (Gu et al., 2011; Marotta et al., 2010). In general, rivers and streams comprise higher pCO_2 than lakes and reservoirs in the same climatic zone, and tropical waters characteristically show higher pCO2 than temperate, boreal, and arctic waters

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(Wen et al., 2021). The pCO_2 in regional and global studies has generally not been measured directly in the field and has been calculated mainly from related parameters like water temperature, pH, and alkalinity measurements or estimated from dissolved organic carbon (DOC) concentration (Cole et al., 1994; Golub et al., 2017). This is very uncertain and leads to substantial errors (Golub et al., 2017). To achieve consistently robust estimates of CO2 emissions from inland waters, future works should concentrate on improving the accuracy and precision of CO2-related parameter measurements as well as direct pCO2 measurements and associated pCO2 calculations (Golub et al., 2017). Some of the above-mentioned pCO2-related parameters can also be derived from satellite data, e.g., lake surface temperature, chlorophyll-a concentration, latitude, CDOM, and solar radiation absorption (Wen et al., 2021). Additionally, optical proxies that can be derived from satellite data have been used to estimate pCO2 indirectly in some rivers and lakes, e.g., CDOM and turbidity index (Kc., 2021; Kutser et al., 2005) have been used. Therefore, in principle, it should be possible to estimate pCO2 in inland waters using satellite-derived parameters.

3.3 Total phosphorus

Inputs of nitrogen and phosphorus to water bodies from catchment areas may lead to eutrophication causing negative ecological changes and can have negative impacts on the use of water for human consumption and as well as for aquaculture production (EEA, 2018). Eutrophication is an ongoing problem in many surface waters of the world and the water quality of surface waters with respect to eutrophication and nutrient concentrations is an objective of numerous directives: the EU Water Framework Directive, the Nitrates Directive, the Urban Waste Water Treatment Directive, the Surface Water for Drinking Directive, and the Drinking Water Directive (EEA, 2018). In

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lakes, the total phosphorus (TP) fraction is generally used as one of the water quality parameters, as long water retention times typically result in only a very small proportion of phosphorus being in the soluble form; the majority being incorporated in planktonic algal cells (Poikane et al., 2019). Therefore, TP (accounts for phosphorus in all the different forms) has been the most widely used phosphor parameter for lakes, mostly measured as annual or growth season means (Poikane et al., 2019). However, the statement that phosphorus alone limits PP in lakes and that reducing phosphorus is enough to control eutrophication (Schindler et al., 2008) has been challenged with evidence that N can play an important role in nutrient limitation of PP in lakes as well (Dolman et al., 2016; Paerl et al., 2018; Poikane et al., 2019). It means that co-limitation is more common than previously assumed and both N and P should be considered as water quality parameters of lakes (Poikane et al., 2019). To support water policy and make informed management decisions, significant resources are expended on producing needful and reliable data to assess and monitor the water quality of surface waters (Lannergård et al., 2019). The selection of the best sampling strategy is critical, which justifies the evaluation of different monitoring methods, use of proxies, and sampling frequencies (Lannergård et al., 2019). Since the lab measurements of nutrients are time-consuming and expensive, more effective methods have been developed. For example, proxies in which low-cost or readily available measurements are used as predictors in transfer functions to predict values (Lannergård et al., 2019). The history of using proxies for estimating the concentrations of water quality parameters dates to 1940s and has been widely used since then (Walling and Webb, 1985). One method for producing high-frequency proxy data appropriate for monitoring water quality is to deploy *in situ* sensors in water bodies to estimate temporal dynamics in the concentrations (Lannergård et al., 2019). High-frequency, *in situ* monitoring can detect time periods and describe trends that may be lost or overlooked by conventional sampling. Unfortunately, many water quality parameters cannot be measured by high-frequency *in situ* sensors due to the

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technological limitations of currently available sensors. However, turbidity is relatively easy to measure *in situ* with high-frequency sensors, and it has the potential to be used as a proxy for other water quality parameters like TP (Al-Ruzouq et al., 2020; Grayson et al., 1996; Jones et al., 2011; Kämäri et al., 2020; Koskiaho et al., 2015; Kusari, 2022; Lannergård et al., 2019; Skarbøvik and Roseth, 2015; Stubblefield et al., 2007). Results from previous studies show significant correlations between turbidity and TP, which indicate that high-frequency turbidity data can be used as a proxy for TP. Although, there might be some limitations. For example, correlations between turbidity and TP seem to be rather site-specific (Grayson et al., 1996; Jones et al., 2011; Kusari, 2022; Lannergård et al., 2019). Unfortunately, studies evaluating the reasons for site-specific correlations are scarce (Lannergård et al., 2019). Additionally, the relationship between turbidity and TP could be affected by sensor maintenance, spatial and diurnal variations, particle size distribution, land management, and the ratio between PO4-P and TP (Kämäri et al., 2020; Lannergård et al., 2019; Pfannkuche and Schmidt, 2003). Though, when doing sensor maintenance and securing data quality the result gives a better more reliable estimate of load and concentrations than when using grab sampling and conventional interpolation methods (Lannergård et al., 2019). It can be concluded, when the aim of environmental monitoring is to describe nutrient loads or status in a water body with high accuracy, using turbidity as a proxy for TP is justified (Lannergård et al., 2019).

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4. *In situ* automated high-frequency monitoring

Until recent decades, the majority of standard lake and coastal monitoring programs were based on manual *in situ* measurements that can be time-consuming (lab analyses may sometimes take days or weeks) and costly to procure. Conventional monitoring often lacks both the necessary spatial coverage as well as an appropriate sampling frequency (Vos et al. 2003). The latter is especially important for detecting the effects of hydrology or weather-related episodic events, from which biological consequences can range from short-term, reversible changes to those that are more persistent (Jennings et al. 2012), as well as using conventional monitoring data for the remote sensing products calibration and validation proposes. Manual monitoring sampling dates are regularly fixed and data collectors do not make changes in their agendas, when the weather conditions are still good enough for sampling (e.g. cloudy or rainy days). This means that collected datasets may not be suitable for remote sensing studies, while satellite images of those days are unusable.

Time and reliability issues can be efficiently addressed by replacing manual measurements with automatic high-frequency measurements (HFM). Many ecosystem processes and water quality changes are far quicker than could be reflected by monthly and even weekly monitoring, therefore only HFM could provide a wealth of data on the natural dynamics of water systems that is impossible to obtain using manual monitoring. Thanks to fast technological development, the autonomy of different measurement systems has increased. Using wireless systems allows retrieving data from the weather and water monitoring stations in near-real time and without manually visiting the study site (Porter et al. 2005). The development of sensors has made progress by taking under consideration the protection from biofouling (Manov et al. 2004) using self-cleaning

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systems (e.g., wipers or pressure). Simple setup of different sensors or just one multi-parametric sonde with a dataloggers enables us nowadays to measure many of the needed water chemical, physical or biological parameters. Some of the first established automated HFM platforms in European lakes (e.g., Lake Erken in Sweden - since 1991 or Lake Feeagh in Ireland - since 2004) record less than hourly changes of lake water physical or chemical changes for many decades (Stokwell et al., 2021). Additionally, to underwater parameters, also air temperature, wind speed and direction as well as solar irradiance data is collected either nearby those systems or on top of the floating platforms. Next sensor setups opened the possibilities to capture also dissolved O_2, pH, electrical conductivity, and turbidity changes in waters. While more and more research institutions and water companies started to use HFM monitoring they also needed to include more and more possible parameters to their systems. Nowadays best equipped HFM platforms are able to detect already tens of different parameters, additionally to the ones mentioned above. Some of the best automated systems are able to detect different phytoplankton pigments fluorescence, organic matter and carbon compounds (CDOM, DOC, pCO2), underwater light fields as well as radiometers to measure radiance, irradiance, or scalar irradiance in the UV, VIS and UV/VIS ranges (https://lexplore.info/). Nowadays weather sensors also include humidity, barometric pressure and precipitation measurements.

The largest advantage of those systems is that they are automated, therefore all the measurements can be made in a pre-specified time frequency and so the data can be collected in all possible weather conditions, which with manual conventional monitoring is impossible or hard to achieve. Having *in situ* measurements close to or exactly on that time when satellite overpass will take place gives us also the best possible opportunities to use this data for remote sensing studies, e.g., calibrating and validating the satellite products.

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It is important that many of the collected datasets have been made available through different internet-based solutions, therefore the data can be used almost in a real-time. Some of the datasets are shared through lake specific web-pages (e.g., Lake Erken, Sweden http://130.238.87.115:8080/ErkenPublic/index.html) some though national environmental data portals (e.g., New Zealand,; https://envdata.boprc.govt.nz/Data) some other through international data initiatives such as EDI or hydroshare (https://portal.edirepository.org, https://www.hydroshare.org). Find additional information about available databases from the Water-ForCE deliverable 4.3.

5. Integrating *in situ* and remote sensing Earth observation for water monitoring

Despite the fact that sensor technology is becoming common in aquatic research and monitoring, current HFM applications focus almost entirely on temporal patterns and variation while spatial variability of aquatic systems is still rarely documented because of the high investment costs for the spatial replication of such infrastructure. Additionally, while this type of infrastructure is costly for many institutions, the number of waterbodies equipped with automated HFM platforms is still small. The Global Lake Ecological Observatory Network (GLEON) combines an array of lake sensors deployed around the globe to address local issues for individual lake ecosystems but also to document changes in lake ecosystems that occur in response to different land use, latitude and climate. As of December 2022, GLEON includes nearly 100 sites equipped with HFM platforms. Considering the large number of individual lakes in the world and

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how many of them we are able to study with *in situ* monitoring techniques, it will be impossible to reach all of the waterbodies and get at least some information about them.

The best, and probably also the easiest, possible option to fill those gaps in the world waterbodies monitoring is to integrate *in situ* monitoring with the satellite earth observations (EO) to increase the number of lakes studied and the knowledge in spatial scale (Siegel et al., 2013, Binding et al., 2018; Hu et al., 2019). EO data provides a frequent, large-scale synoptic overview of lakes and has increasingly been integrated operationally into inland water monitoring (Binding et al., 2021). Currently, there are no satellite sensors which specifically address all challenges related to coastal, and particularly, inland water remote sensing. Instead, satellites that have been designed for other purposes (e.g., land or open ocean remote sensing) have to be used. However, it has been demonstrated that data from different ESA (European Space Agency), NASA (The National Aeronautics and Space Administration) and other space agencies satellites can be used to detect several inland water parameters (Palmer et al. 2015, Toming et al., 2016a, Ansper & Alikas, 2018; Bonansea et al., 2019; Page et al., 2019; Al-Kharusi et al., 2020). The European Union's Earth Observation Programme Copernicus currently provides data access to up to four satellites to derive optical water quality parameters in lakes. Sentinel-3 (S3) Ocean and Land Colour Instrument (OLCI) offers an opportunity to monitor inland and coastal waters with high spectral (21 bands) and temporal (global coverage every two days) resolution. Still, it is more suitable for monitoring large water bodies because of its spatial resolution (pixel size 300 m on the ground). Another ESA satellite Sentinel-2 (S2) Multispectral Instrument (MSI) allows monitoring of smaller water bodies, with spatial resolution of 10-60 m on the ground, but has lower spectral, radiometric and temporal resolution compared to Sentinel-3 OLCI. Although Sentinel 2 was initially created for land applications, water quality parameters can be still successfully mapped (Toming et al., 2016a, Ansper & Alikas, 2018, Al-Kharusi et al., 2020).

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The Copernicus Land Monitoring Service (CLMS) already provides some lake water related products through the continuous observation record for a large number (nominally 4,200 for water quality) of medium and large-sized inland water bodies (lakes, reservoirs, and some lagoons and riverine wetlands). Within the list of datasets from CLMS the following water quality related products are available:

- Lake Surface Water Temperature
- Lake Water Quality 100 m (restarted in 2022)
- Lake Water Quality 300 m
- Lake Water Quality 1 km (discontinued)

All those and many other current Copernicus products are described in more detail in Water-ForCE deliverable 2.2 “Analysis of current Copernicus water quality portfolio” report. All those products have been tested for reliability and can be used for country or region-based lake state monitoring. Working out new possible higher-level products between *in situ* and satellite based EO data enables us more accurate near-real time monitoring for future.

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6. Conclusions and recommendations

With the current document we would like to raise awareness about possibilities of new water related higher-level products for the future Copernicus water related services. This report proposes, based on user's requirements, that mass primary production, concentration of dissolved organic carbon, partial pressure of carbon dioxide and concentration of total phosphorus can be estimated using other *in situ* measurement techniques or proxy parameters from automated HFM. We see that many of those parameters can be directly obtained from the remote monitoring and therefore could be easily accessible also from Copernicus EO satellites data.

Still, to get the best possible new products in case of reliability and accuracy, both *in situ* and remote sensing networks should work together. First, it is important that the *in situ* data collection would happen at the appropriate time (e.g. close to the satellite overpass and with clear weather), so that collected datasets would be also usable for remote sensing studies. Secondly, to increase the reliability and accuracy of both *in situ* and remote sensing monitoring results, more frequent data collection is needed. This can be achieved using more automated monitoring systems in waterbodies. It would be the best if some of those HFM systems could be also equipped with exactly those sensors (e.g. fDOM, $CO2$, reflectance) which variables are needed to build up the offered new higher-level products, and if possible also with a sensor for global irradiance and reflectance measurements. Thirdly, all those datasets should be made openly available following the FAIR principles, so they could be used for all possible communities (e.g. for calibrating their products). Finally, all the already existing and future higher-level products need maximum validation, this means that the amount of *in situ* data collection should never decrease. Achieving all of this we will result in larger knowledge about the status of waterbodies on Earth.

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