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Retrieving water chlorophyll-*a* concentration in inland waters from Sentinel-2 imagery: Review of operability, performance and ways forward

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A R T I C L E I N F O

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A B S T R A C T

The fundamental role of water for life and the threats to water bodies around the world have highlighted the need for their conservation. Remote sensing is a tool that allows us to monitor water bodies in a rapid, systematic, accurate and economical way, being complementary to traditional field sampling methods. The main aim of this review is to synthesise the use of the Sentinel-2 satellite for chlorophyll-a monitoring, an indicator of the trophic state of aquatic ecosystems, and assess the role of each parameter on chlorophyll-a retrieval. To this end, indices, models, atmospheric corrections and field sampling details used so far in chlorophyll-a monitoring of aquatic ecosystems using Sentinel-2 imagery were analysed. Sentinel-2 was chosen because it has suitable features for monitoring water bodies (spatial, temporal and spectral resolution), despite not having been specifically designed for that purpose. The indices aphy(B4)/a*phy(B4), B7(1/B4-1/B5), B5-(B6 + B4)/2 and B3/B4 performed best in lakes and B2 + B3 + B4 + B5, B3/B6 and (B5-B4)/(B5 + B4) in reservoirs. The atmospheric correction ELM performed worse than Sen2Cor and ATCOR in lakes. In reservoirs, ATCOR performed best and C2XC and Dark Object Subtraction performed worse. Finally, classical machine learning and deep learning models outperformed traditional linear and non-linear models. An integrated vision of remote sensing with Ecology could improve some weaknesses found in the reviewed articles, such as the lack of methodological details in field sampling or knowledge of the dynamics and functioning of the ecosystem to achieve the most optimal sampling of the system. By doing so the field of remote sensing would have a higher aplicability. Some further investigations are needed on small water bodies (area < 0.1 km^2), which have been scarcely studied by remote sensing, although accounting for >90% of the water bodies worldwide.

1. Introduction

Water plays a key role in social and ecological systems as a source of life, primary production, income, goods and services. However, aquatic environments are facing increasing threats due to environmental stressors that affect both water availability and quality and aquatic ecosystem functioning (UNESCO, 2015). Water availability and quality have been prioritised by international policies such as the 2030 Agenda and the Sustainable Development Goals. Thus, there is an urgent and increasing need for monitoring and managing water ecosystems in a rapid, systematic, comprehensive, accurate and economically feasible way. Continuous data on biological and physicochemical parameters of water ecosystems are generally lacking for most water bodies and have traditionally been monitored by field sampling (Filazzola et al., 2020), which has however some limitations: (a) field sampling and subsequent laboratory analyses require high human and economic resources, (b) some water bodies are hardly accessible (Gholizadeh et al., 2016), which makes their regular space-time monitoring very difficult or almost impossible. Satellite remote sensing represents an opportunity to overcome some of these limitations thanks to the constantly growing temporal, spatial and spectral coverage of the new sensors being launched. This, together with the increasing volume of remote sensing images and

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the opportunities offered by new-generation satellites has led to an extensive application of remote sensing to the monitoring of aquatic environments and to several hydrological applications (Topp et al., 2020). Nevertheless, remote sensing technology is not expected to replace, but to be complementary to field sampling, which is still essential, since (1) it provides training and calibration data for remote sensing models, (2) the current spatial, spectral coverage and temporal resolution of freely accessible satellites is not yet able to cover the needs of all the water bodies, especially the smallest and shallowest ones, and (3) remote sensing alone cannot fully assess aquatic ecosystem properties and processes.

Water monitoring studies can be divided into two main categories: assessment of water quantity and of water quality, focusing this review on the second one. Water quality parameters such as chlorophyll-*a* (chl-*a*), coloured dissolved organic matter (CDOM), and total suspended solids (TSS) have been widely estimated by remote sensing, as they are optically-active substances with distinctive spectral signatures (Abdelal et al., 2022; Zhang et al., 2017). Chlorophyll-*a* is the most commonly measured parameter in water quality studies (i.e. see Cillero Castro et al., 2020; Jaelani and Ratnaningsih, 2018), as it is a direct proxy of algal biomass concentration (Cullen, 1982) and an indicator of the trophic status of the water (OCDE, 1982), which links nutrient concentration and algal biomass and primary production. However, some uncertainty is expected owing to each cell type, algae species or even the physiologic state of the cells may contain different concentrations of chl-*a* (Reynolds, 1984).

Remote sensing of water bodies has been widely applied to oceanic ecosystems since the 1970s. Indeed, chlorophyll-*a* was first derived using remote sensing in 1974 in oceans using ocean colour satellites (Matthews, 2011). Most studies on inland water bodies started in the 1990s and have considerably increased since the 2000s (Hestir et al., 2015). By digging into this literature, we became aware of the general shortage of an ecological perspective in the interpretation of the results. A technical perspective alone in the pursuit of chl-a satellite monitoring may leave relevant ecological processes behind.

Remote sensing application in inland aquatic environments began with sensors specifically conceived for ocean studies, known as ocean colour sensors, such as MODIS, SeaWIFS, OCM and MERIS, whose technical characteristics (see Supplementary Table S1) are optimal for the study of water constituents in marine waters. However, the spatial resolution of the different satellite missions has been traditionally a limiting factor for the monitoring task of freshwater ecosystem properties and processes (Hestir et al., 2015). MERIS, with a spatial resolution of 300 m, and MODIS, with a spatial resolution of up to 250 m, have been widely used for water-component retrievals in coastal and inland waters, allowing long-term time series and long-term monitoring, but just on very large aquatic ecosystems (Matthews, 2011).

New opportunities emerged with the latest generation of multispectral sensors, including Landsat-8 OLI (Operational Land Imager), Sentinel-2 MSI (Multispectral Instrument), and Sentinel-3 OLCI (Ocean and Land Colour Imager Sensor) (see Supplementary Table S1). This new generation of sensors offers a finer temporal, spatial and radiometric resolution than its predecessors, opening the possibility of analysing much smaller water bodies (Toming et al., 2016) and monitoring short-term processes and dynamics (Pinardi et al., 2018). Despite being designed for land monitoring purposes, they have shown good performance in several inland and transitional waters studies, although their spectral coverage and spatial resolution may limit the detection and analysis of certain water constituents and make the use of certain atmospheric correction models difficult (Matthews, 2011), which is a crucial step in remote sensing studies since atmospheric gases and aerosols influence the reflectance captured by satellite sensors (IOCGG, 2010).

The Sentinel-2 mission, within the Copernicus Missions of the European Space Agency (ESA), comprises two twin satellites phased 180° to each other: Sentinel-2A and Sentinel-2B launched in June 2015 and March 2017, respectively. Both Sentinel-2 MSI sensors reach a high temporal resolution with a combined revisit time of up to five days on average at mid-latitudes, a high spatial resolution ranging from 10 to 60 m depending on the spectral band, and a high spectral coverage with 13 spectral bands covering the visible (VIS), near-infrared (NIR), and shortwave infrared (SWIR) bands (European Space Agency, 2015). They include key bands for the study of aquatic ecosystems such as the red-edge band at 705 nm which is the most significant band for phytoplankton bloom determination (Kutser et al., 2016), as many cyanobacteria cause a reflectance peak near 700 nm, making it suitable for the development of chlorophyll-*a* retrieval algorithms in water bodies. In this context, Sentinel-2 (referring both to Sentinel-2 A and B hereafter) was chosen for this review, despite being designed for land monitoring, as it has also been proved to have the ideal combination of spectral bands and temporal and spatial resolution for the monitoring of water masses (e.g. Beck et al., 2016; Pereira et al., 2020) and its spatial resolution of up to 10 m allows the remote monitoring of relatively small water bodies.

The main objective of this article is to review, from an ecological and technical perspective, the retrieval of chlorophyll-*a* concentration in the water column of aquatic ecosystems by means of Sentinel-2 imagery. To do so, the specific objectives of this article are to provide: (a) a review of the spectral indices, atmospheric corrections, and modelling approaches used in the literature to measure chlorophyll-*a*, and (b) a synthesis of the best practices and future opportunities offered by remote sensing for chlorophyll-*a* retrieval.

2. Methodology

2.1. Literature search

We conducted a systematic literature search using Web of Science (WoS) (at: https://webofknowledge.com/) and Scopus (at: https://www.scopus.com/) core search engines. The literature search included all works published until the end of December 2022. The search focused on the use of Sentinel-2 imagery for chlorophyll-a concentration retrieval in water bodies. Inland and coastal water systems were the focus of this review. However, this topic was not included in the search to avoid missing relevant articles given the high number of denominations given to different aquatic systems. Then, studies on open oceanic waters environments were manually removed after reading each article. The following search string was used: TITLE, ABSTRACT OR KEYWORDS = ("chlorophyll*" OR "chl*") AND ("sentinel-2" OR "sentinel2" OR "sentinel 2" OR "MSI") AND publication date = 2015–2022.

As a result, a total of 1,412 (last search conducted on 17th January 2023) unduplicated articles, reviews, book chapters and conference proceedings were obtained. To exclude studies that were not in the scope of this review, each document was individually read to avoid those focusing on terrestrial and riparian vegetation chlorophyll, those merely mentioning the Sentinel-2 imagery but not really using it, and those using simulated data instead of actual Sentinel-2 data. Finally, a total number of 137 articles using Sentinel-2 bands to detect chlorophyll-*a* from the water column were included in this review.

2.2. Information extracted from the articles

The publications were annotated using the following criteria: objective of the reviewed studies, chlorophyll-*a* retrieval indices, atmospheric correction models, chlorophyll-*a* models, water system characterisation (geographical location, ecosystem type and size of the water body) details about field sampling (Table 1) and the used methods for measuring chl-*a* concentration.

Spectral indices are combinations of spectral bands that correlate well with the desired ecological variables, which in this study is the chl-*a*. They take the values from different regions of the spectrum and

Table 1
Selected key information extracted from the reviewed studies, levels assigned to each one and description about the levels, when applicable.

Criteria	Levels to the criteria	Description of the levels
Objective of the study	Assessment of satellite, model, and index performance	Feasibility of Sentinel-2 imagery and performance of several indexes or models to estimate chlorophyll-*a*
	Effect of atmospheric correction (AC)	Performance of AC models or comparison among several for the retrieval of chlorophyll-*a* concentration
	Assessment of water quality	Assessment of Sentinel-2 models for the determination of the trophic state of the water, the spatio-temporal evolution of water quality parameters (chlorophyll-*a*, nutrient concentration, …) or for the monitoring of harmful algal blooms
	Effect of field-to-satellite time span	Effect of the time span between the field and satellite sampling
	Aquaculture production	Feasibility of Sentinel-2 to improve or monitor aquaculture production
	Effect of disturbances	Assessment of the effect of a specific perturbation on the chlorophyll-*a* concentration of a given ecosystem
Chlorophyll-*a* indices	Criteria not levelled. It was noted with the original names from the source study.	
Atmospheric corrections	Criteria not levelled. It was noted with the original names from the source study.	
Models	See supplementary Table S3	
Region of study	Levelled by countries	
Ecosystem type	Lake	
	Reservoir	
	River	
	Coast (neritic ecosystems)	
	Estuary	
	Combination	
Field sampling methodological aspects	Time window between sample collection and satellite overpass	
	Distance from the shore	
	Depth at which the sample was collected and	
	Depth of the water column at the sampling point	
Methodology for chl-*a* measurement	Criteria not levelled. It was noted with the original names from the source study.	Methodology for chl-*a* measurement in the laboratory

provide a specific value, which then will be used to derive our interest information. In some cases, this will be done by the application of different models, which are mathematical relationships between spectral indices and field-estimated chl-*a*.

To compare and rank the performance of the spectral indices used in the literature to estimate chlorophyll-*a* from Sentinel-2, we first annotated both the used Sentinel-2 bands (either if explicitly provided in the study or by proximity of the specified wavelength to each Sentinel-2 band) and their original formula (Supplementary Table S2). We excluded multiplicative weighting factors or adjustments applied in specific study areas to avoid considering variations of the same index when summarising the frequency of their use. Second, we recorded all statistical goodness of fit and error estimates obtained from the literature. The different models used in the analysed literature were grouped into different categories to simplify their analysis. The details of this classification can be found in the Supplementary Table S3. To know what models and indices provide better performance to estimate chlorophyll-*a* across all studies, we recorded and compared all goodness of fit and error estimates provided in each study. As an exception, we did not use the Root Mean Square Error (RMSE), as it is a statistical parameter highly dependent on the order of magnitude in the data. Thus, it is useful when comparing within the same dataset but should be avoided to compare between different datasets with different scales (Hyndman and Koehler, 2006).

2.3. Statistical analysis

Generalized linear models (GLM) were performed to compare the performance of the analysed parameters for each ecosystem type. We used R^2 as a comparative metric since it was the most used among all articles and our ability to compare the performance of the methods used in the different articles was limited, as methods and goodness of fit evaluation strongly differed among studies. As R^2 is bounded between 0 and 1, the quasibinomial family was used for the GLM analysis. To test the performance of sample depth collection, chl-*a* measurement methodology, sample collection depth, models, and atmospheric correction models, all the comparisons possible were tested. To test the indices performance, GLM analyses were performed taking the most widely used (used in 3 or more study cases) and best performing (based on mean R^2 value) indices for each ecosystem (Supplementary Table S4) as reference values to compare the performance of the whole index pool to these both selected indices.

3. Results and discussion

A total of 1,412 articles appeared in the bibliographic search, of which 137 were relevant for this review. The multiple combinations among atmospheric corrections and spectral indices impeded the independent comparison of performance among these two factors, as chl-*a* retrieval is a function of the atmospheric correction along with the bio-optical indices used and that there is no reliable way to decouple them when assessing performance. For instance, a maximum of 17 out of 137 articles used the same atmospheric correction and spectral index in the same ecosystem type (see Supplementary Table S5) and a maximum of 32 out of 137 articles used the same atmospheric correction and spectral index when comparing the articles as a whole (see Supplementary Table S6).

3.1. Goals of the reviewed publications

Assessing the performance of the satellite sensor and of different models and indices was the most common goal of the reviewed studies, followed by the water quality assessment (60 % and 25 % of studies, respectively) (Supplementary Figure S1). The least frequent goals were aquaculture purposes and the time window effect assessment (3 % and 1 %, respectively).

The assessment of the satellite feasibility and model and index performance was the predominant study objective across system types, except for the estuaries, followed by the assessment of the water quality (Fig. 1). The assessment of the performance of different atmospheric correction models was among the main study objectives in all ecosystem types. The assessment of the effect of a disturbance has been conducted in lakes, reservoirs, and rivers, being one of the main objectives in rivers. Finally, the effect of the time window between the satellite overpass and the field sampling and the assessment of using Sentinel-2 for aquaculture purposes have been studied only in reservoirs and coastal areas, respectively.

Under the current scenarios of climate change, water pollution and increasing demand for water resources, most of the water bodies have experienced a decline in their water level and/or water quality (Mekonnen and Hoekstra, 2016). Thus, water quality assessment evaluation is one of the main objectives in lakes and reservoirs, which are the

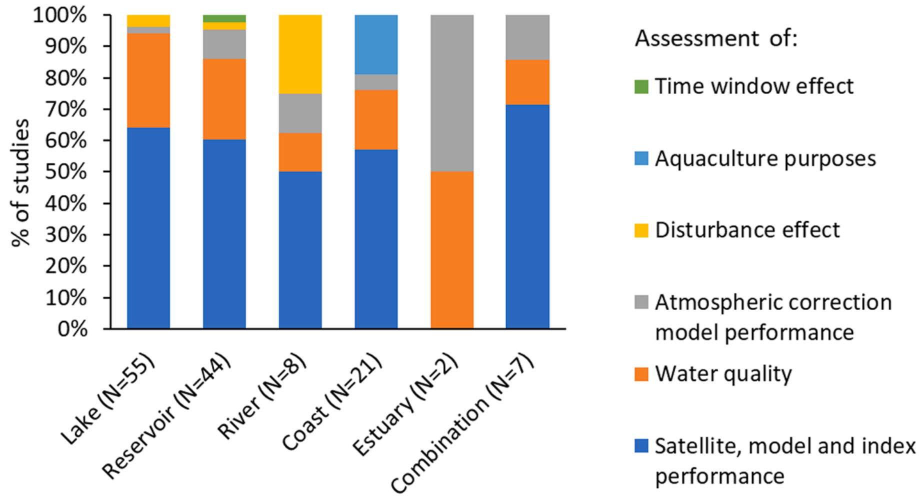

Fig. 1. Distribution of the main objective of the reviewed studies (total count of studies = 137) obtained from Scopus and Web of Science that used Sentinel-2 satellite data to assess chlorophyll-*a* concentration in continental and coastal waters between 2015 and 2022 sorted by studied ecosystem type.

main sources of drinking water, water for agriculture purposes, etc. Among the studies on water quality, many of them are dedicated to the assessment of harmful algal blooms (HABs), which are a source of toxins making water unsafe to drink (Aubriot et al., 2020). These HABs have been treated as the main objectives in studies in coastal zones which are suffering increasing eutrophication representing a potential risk for beachgoers (Ivanda et al., 2021) and for aquaculture activities carried out in these areas.

3.2. Spectral indices: Use and performance to estimate chlorophyll-a

Spectral indices are combinations of spectral bands that correlate well with the desired ecological variables. The statistical parameter R^2 was used to compare the indices performance as it was the most widely used. The full set of indices and their statistical parameters are available in the Supplementary Table S7.

Statistically significant results of the GLM analysis were obtained only for lakes and reservoirs. In lakes, selected reference indices performed mainly better than the comparison indices (Fig. 2). In reservoirs, two of the five selected indices performed worse than the comparison ones (Fig. 2). In all the other ecosystems indices performance showed no significant performance difference in comparison to the reference ones.

In lakes, it is noteworthy that the indices performing worse than the reference ones are repeated for all the reference ones. Most of these indices contain the bands 1, 2, 3 and 8. In lakes, indices (B1/B2-B2/B3)/(B1/B2 + B2/B3), (B1 + B2)/(B4/B2), B6*(1/B5-1/B4) and B8/B4 performed worse than any reference index (Supplementary Table S8). The index B4/B5 is the most widely used in lakes (N = 20), as the slope between bands 4 and 5 has been identified as the most sensitive to changes in chlorophyll-*a* concentration, regardless of the atmospheric correction used (Zabaleta et al., 2021). The performance of these bands (665 and 705 nm, respectively) might be explained by the absorption peaks of chlorophyll-*a* in the red part of the spectra at around 665 nm, whereas water absorption peak is at around 708 nm. However, the index B4/B5 in lakes and the index B5/B4 in reservoirs are outperformed by other indices (Table 2). In reservoirs, the index (B3-B2)/(B3 + B2) performed worse than three of the reference indices and B5-(B6 + B4)/2 performed worse than two of them.

The application of remote sensing in coastal and inland waters (referring to Case-2 waters according to the classification made by Morel and Prieur (1977) might not be straightforward as they have a complex composition containing a wide range of optically active constituents (OAC). Monitoring coastal and inland waters is especially challenging due to the adjacency and bottom effects, as these water bodies tend to be shallow and/or small, and due to the high amount of optical water types having a predominance of chlorophyll-*a*, CDOM, TSS or any combination among them and other water components. The adjacency effect is the effect of the adjacent land pixels (Pan et al., 2022), whereas the

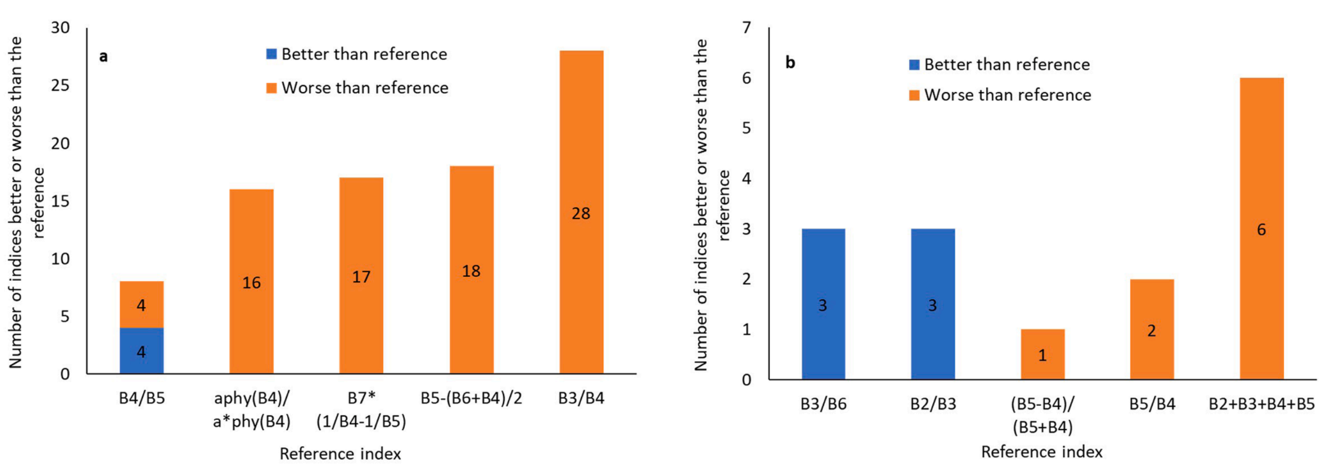

Fig. 2. Number of indices performing significantly better or worse than the reference indices in (a) lakes and (b) reservoirs. [1] aphy = absorption coefficient of phytoplankton. For more information see original reference Gons *et al* (2005).

Table 2
Atmospheric correction model performance comparison through GLM results analysis. (<) and (>) represent the better or worse performance, respectively, of a comparison AC model in comparison to the reference AC model. (**) indicates a significant performance difference (p-value < 0.05) and (*) indicates marginal significance (p-value < 0.1). (n.s.) indicates no significant performance difference between AC models.

	Reference AC model	Sign and significance of comparison	Compared AC model
Lake	ELM	< **	Sen2Cor
		<**	ATCOR
Reservoir	ATCOR	> *	Sen2Cor
		>**	iCor
		>**	Dark Object Subtraction
		>**	C2XC
	C2XC	< **	Sen2Cor
		<**	ATCOR
		<**	6S
		<*	Acolite_DSF
		<**	SeaDAS
	Polymer	> *	Dark Object Subtraction
		>**	C2XC
	SeaDAS	> **	Dark Object Subtractioni
		>**	iCor
	Dark Object Subtraction	< *	Sen2Cor
		<**	ATCOR
		<**	6S

bottom effect takes place when the sediment or benthic communities' reflectance exceeds the water absorptive properties, especially in the near and shortwave infrared wavelengths (Topp et al., 2020). Relatively small, temporally dynamic and spatially and optically complex water bodies require higher temporal, spatial and spectral coverage, higher atmospheric correction accuracy and the application of additional water inherent optical properties (IOP) retrieval algorithms (IOCGG, 2010). In this complex ecosystem, including the blue band (Sentinel-2 band 2; 495 nm) may be challenging in cases where chlorophyll-*a* and CDOM absorption in the blue band overlap. In fact, the blue band was not included among the best-performing indices for lake and coastal ecosystems determined in this review. In these cases, the use of the NIR band (Sentinel-2 band 8; 835 nm) has performed well and might overcome this shortcoming. Indeed, the NIR band was included in the best-performing indices of lacustrine and coastal ecosystems. Kutser et al. (2016) found that the most useful wavelengths for the retrieval of chlorophyll-*a* and total suspended matter concentrations was 710 nm (most appropriate Sentinel-2 band 5; Red Edge1; 704 nm) in productive waters and 810 nm (most appropriate Sentinel-2 band 8; NIR; 830 nm) in extreme cases with a high predominance of CDOM in which its absorption is still high at 710 nm. In coastal turbid waters the spectral water-leaving radiance reflectance is poorly sensitive to changes in chlorophyll-*a* concentration (between 400 and 580 nm) thus discouraging the use of models including wavelengths within this range Gernez et al. (2017). The accuracy of the NIR/Red (Sentinel-2 bands 8 and 4; 835 and 665 nm) index decreases in cases in which the chlorophyll-*a* concentration is too low. In this case, it is advisable to shift to the blue/green (Sentinel-2 Bands 2 and 3; 496 and 650 nm) part of the spectra (Gernez et al., 2017). Besides, the presence and even dominance of CDOM could limit the use of models created for oceanic ecosystems in coastal and inland waters or might require some modifications. Knowing the predominant OAC is thus essential for the selection of the best model, as done by Soomets et al. (2020) and Uudeberg et al. (2019), where water bodies of their study area were classified under the frame of the optical water type (OWT) (Morel and Prieur, 1977) according to the dominance of chl-*a*, TSS or CDOM in the study system, and the best index was subsequently selected for each type.

The best index for different water systems can also be selected according to the chlorophyll-*a* range such as in (Sòria-Perpinyà et al., 2021), showing that each band combination has a range of chlorophyll-*a* concentration in which it performs best. Also, coastal and inland waters might present a dynamic change over time, thus requiring different remote sensing models throughout the year (Cairo et al., 2020), as the models including the seasonal effect have shown better performance in the prediction of the chlorophyll-*a* concentration (Elhag et al., 2021). However, others found that the same model had a similar performance regardless of the season of the year (Shi et al., 2022).

3.3. Atmospheric corrections: Trends in their use and performance

The atmospheric correction is a crucial step in remote sensing studies since the influence of gases and aerosols present in the atmosphere are captured by satellite sensors (IOCGG, 2010) making it difficult to determine what percentage of the signal is attributable purely to water and its optically active constituents (OAC). Despite the significance of this fact, among the reviewed studies, only nine were specifically related to the atmospheric correction assessment.

The use of level-1C Sentinel-2 images (i.e., non-atmospherically corrected or Top Of Atmosphere images; TOA) and images corrected through the Sen2Cor atmospheric correction was predominant (Fig. 3). Sen2Cor was initially created for land purposes, but it has also been used successfully for water purposes (Pereira-Sandoval et al., 2019). In this regard, many articles such as Nguyen et al. (2020) and (Sòria-Perpinyà et al., 2019) used Sen2Cor for the correction of S2 images for turbid and hypereutrophic waters, respectively. However, it did not always show a good performance in all water ecosystems (i.e. Dörnhöfer et al., 2016; Toming et al., 2016; Xu et al., 2019) and it has been proven to be inappropriate for the estimation of reflectance within the near infrared (NIR; Sentinel-2 Band 5) (Thi Thu Ha et al., 2017). The different AC models might have a heterogeneous effect on the different bands, especially on the longer wavelength bands most commonly used in chl-*a* retrieval (S2 Bands 4, 5 and 6) (Grendaitė and Stonevičius, 2021). However, Sen2Cor might be the most widely used over time, probably because it is the default atmospheric correction for Sentinel-2 and is available in most satellite image processing software, so its use is very straightforward and no additional knowledge is required. TOA images were still commonly used, probably because TOA images perform better than images atmospherically corrected under certain circumstances (Barraza-Moraga et al., 2022). Also, TOA images are a good alternative in cases when there is no available in situ data (Grendaitė and Stonevičius, 2021) to perform the AC.

The use of machine learning-based AC models is increasing over time showing an improved performance over non-machine learning-based ones (Supplementary Table S9 for classification details). Since 2019 onwards the use of these machine learning-based AC has been implemented and it has been rising. For instance, in 2019 ACOLITE_DSF (Atmospheric Correction for OLI Lite), C2RCC (Case-2 Regional Coast Color) and C2X (Case-2 Extreme Waters) began to be used. The ACOLITE AC algorithm, originally created for water purposes, performed well in inland water bodies, especially in the blue-to-red region of the spectrum, although needing some improvements in the NIR region (Warren et al., 2019). It has the advantage of including a correction for the sun-glint (Tavares et al., 2021). C2RCC is a machine learning AC model that has been shown to outperform in very clear or ultra-oligotrophic waters (Radin et al., 2020), although it showed some performance deficiencies

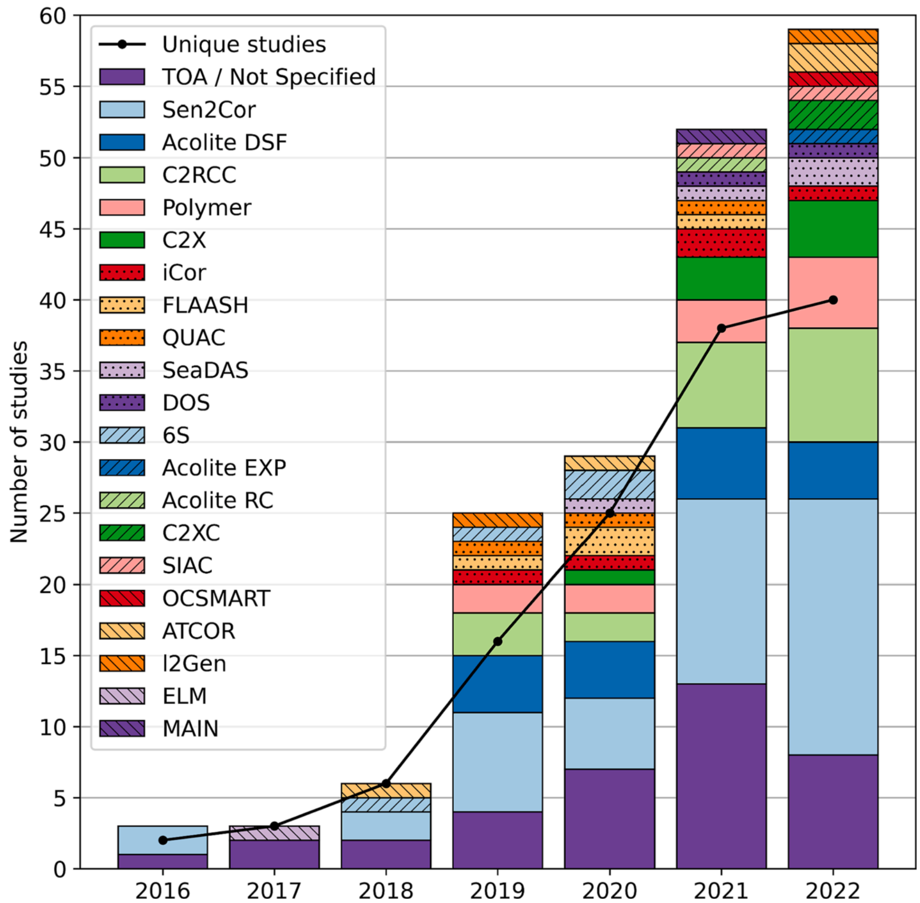

Fig. 3. Number of reviewed studies that used Sentinel-2 satellite data to assess chlorophyll-*a* concentration in continental and coastal waters between 2015 and 2022 that used each atmospheric correction model over the years. The total number of studies represented by bars might be higher than the total number of reviewed studies, as some of them used several AC models and were counted more than once when it was used several times in the same article or when an article used different ones. The total number of studies published each year is indicated by the black line. Long names of atmospheric corrections (when available): Case-2 Regional Coast Color (C2RCC), Atmospheric Correction for OLI Lite (ACOLITE), Dark Spectrum Fitting (DSF), Polynomial based algorithm applied to MERIS (POLYMER), Case-2 Extreme Waters (C2X), Image Correction for Atmospheric Effects (iCor), SeaWIFS Data Analysis System (SeaDAS), Fast Line-of-sight Atmospheric Analysis of Hypercubes (FLAASH), Second Simulation of the Satellite Signal in the Solar Spectrum (6S), Atmospheric and Topographic Correction (ATCOR), Quick Atmospheric Correction (QUAC), Dark Object Subtraction (DOS), Case-2 Extreme Waters Complex (C2XC), Sensor Invariant Atmospheric Correction (SIAC), Ocean Color-Simultaneous Marine and Aerosol Retrieval Tool (OC-SMART), Empirical Line Method (ELM) and Modified Atmospheric Correction for Inland Waters (MAIN) and not corrected satellite images (Top of Atmosphere - TOA).

in the red region of the spectra (Sentinel-2 band 4; 665 nm), which can cause the miss of the chlorophyll-*a* absorption peak at this wavelength (Soomets et al., 2020). C2X was selected as the best atmospheric correction in different lakes located in the German lowlands (Ogashawara et al., 2021). C2X atmospheric correction has performed especially well for the red and NIR-red edge bands (Virdis et al., 2022) and outperformed both in clear waters (Soomets et al., 2020) and in turbid waters with high phytoplankton concentrations (Radin et al., 2020). While artificial intelligence-based models are on the rise, the use of traditional models is declining. For instance, FLAASH (Fast Line-of-sight Atmospheric Analysis of Hypercubes) and QUAC (Quick Atmospheric Correction) stopped being used in 2022. The FLAASH AC was originally created for land applications and has the disadvantage of not correcting for the sky reflectance, thus giving overestimated results (Cao et al., 2021). It is, however, noteworthy that the traditional AC model (not based on machine learning) iCor is the only AC model correcting for the adjacency effect (Warren et al., 2019).

Among all the ecosystem types, the most widely-used atmospheric correction (AC) models were Sen2Cor, ACOLITE, C2RCC and Polymer (Polynomial based algorithm applied to MERIS), although the non-use of AC has been seen to be predominant across most of the ecosystems studied, except for the marine ecosystems (Fig. 4). POLYMER is an atmospheric correction algorithm originally created for oceanic systems and it has shown a very good performance due to the specific correction for the sun-glint effect (Warren et al., 2019).

The selection of an AC becomes less important when the chlorophyll-*a* concentration is retrieved through shorter wavelengths and its importance depends on the chlorophyll-*a* model used, as some have a higher influence from the AC (Grendaitė and Stonevičius, 2021). The most commonly used Sentinel-2 bands for chlorophyll-*a* retrieval: band 4 (665 nm), band 5 (705 nm) and band 6 (740 nm) are the most variable and show a high uncertainty according to the AC algorithm used (Grendaitė and Stonevičius, 2021). Thus, simplified atmospheric corrections should be prioritised, as more complex atmospheric corrections (e.g., for aerosols) might generate errors in water bodies with high turbidity and high biomass content (Barraza-Moraga et al., 2022).

In fact, the number of parameters that interfere with the process of satellite detection of water constituents might be high in coastal and inland waters, as they might be affected by bottom and adjacency effects. That makes the ideal atmospheric corrections for the coastal ecosystems uncertain thus requiring more research, especially for the smallest and shallowest ecosystems (Soriano-González et al., 2019).

GLM analysis shows major significant differences in AC models performance in lakes and reservoirs (Table 2). C2XC and Dark Object

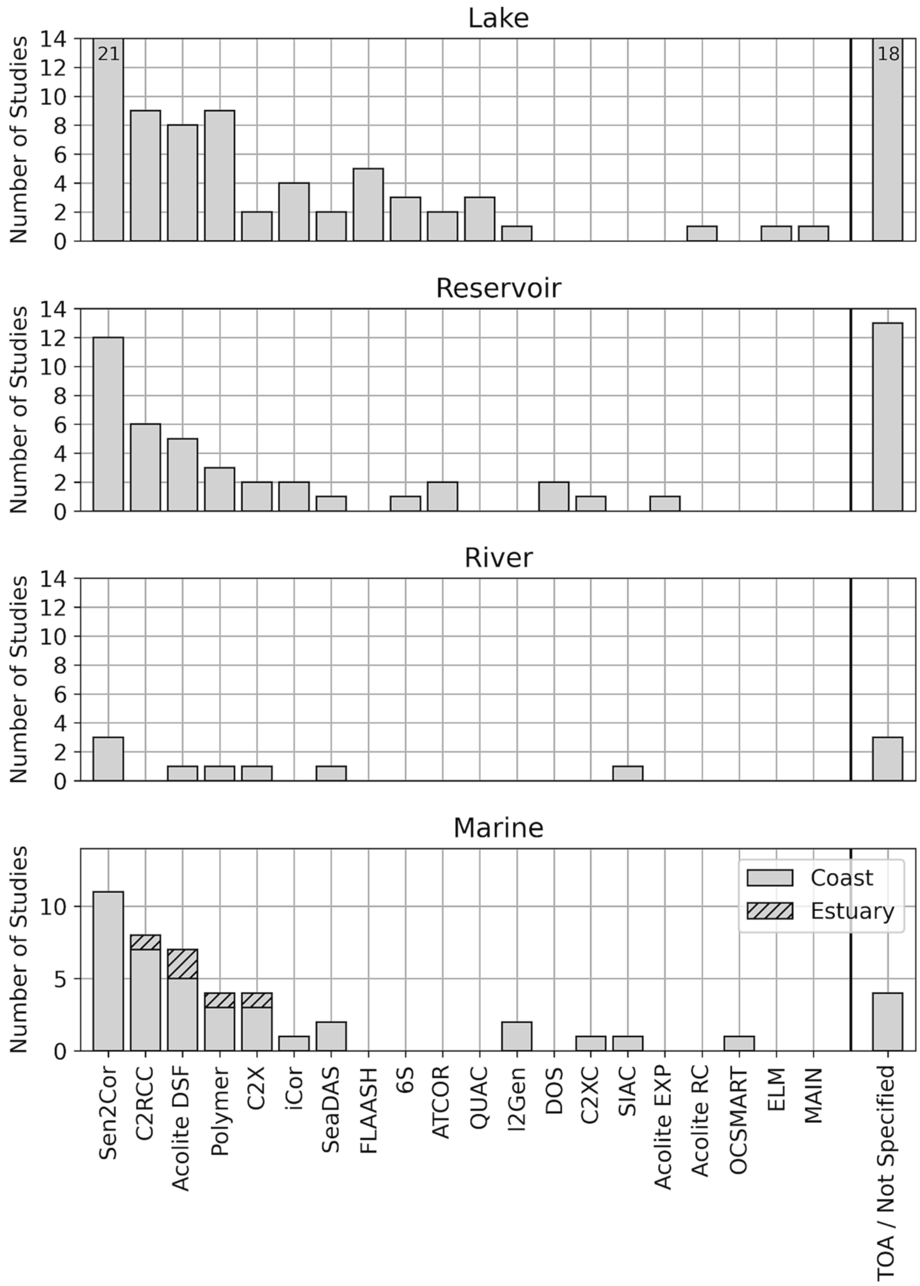

Fig. 4. Number of reviewed studies that used each AC model sorted by system type. Acronyms are detailed in Fig. 3.

Subtraction were the worst performing AC models in reservoirs performing worse than Sen2Cor, ATCOR, 6S and ACOLITE_DSF and worse than Sen2Cor, ATCOR, 6S, SeaDAS and POLYMER, respectively. On the other hand, ATCOR outperformed Sen2Cor, iCor, Dark Object Subtraction and C2XC. In lakes, ELM performed significantly worse than Sen2Cor and ATCOR. A worse performance of ELM in comparison to Sen2Cor and ATCOR was also seen in lakes. A full list of the AC models and their associated goodness of fit parameters can be consulted in the Supplementary Table S10. No significant statistical differences between AC models were detected for rivers, coasts nor estuaries.

3.4. Models: trends in their use and performance

The reviewed models refer to mathematical relationships between spectral indices and field-estimated chl-*a*. Classical linear models were predominantly used in the literature, although their use has decreased over time (Fig. 5). The use of non-linear models was generally stable in time, being representative among the models, although not predominant. Physics-based models were the least used, having their highest utilisation rate in 2021. On the contrary, the application of machine learning techniques, both classical machine learning and deep learning, experienced a rise. These models rely less on atmospheric conditions and might overcome the common non-linearity between satellite spectral bands and field data and they have been seen to overcome traditional linear models, especially in low chlorophyll-*a* water bodies (Q. Cao et al., 2022).

One of the most widely used models, the classical machine learning model Extreme Gradient Boost (XGBoost) uses a methodology, which helps to improve the generalisation performance of the model and prevent overfitting, making it ideal for solving complex non-linear regression problems (Tian et al., 2022). Nonetheless, XGBoost and other classical machine learning models such as Random Forest (RF) tended to overestimate the chlorophyll-*a* values with a low concentration (<15 μg/L) and slightly underestimate the Chl-*a* values with a high

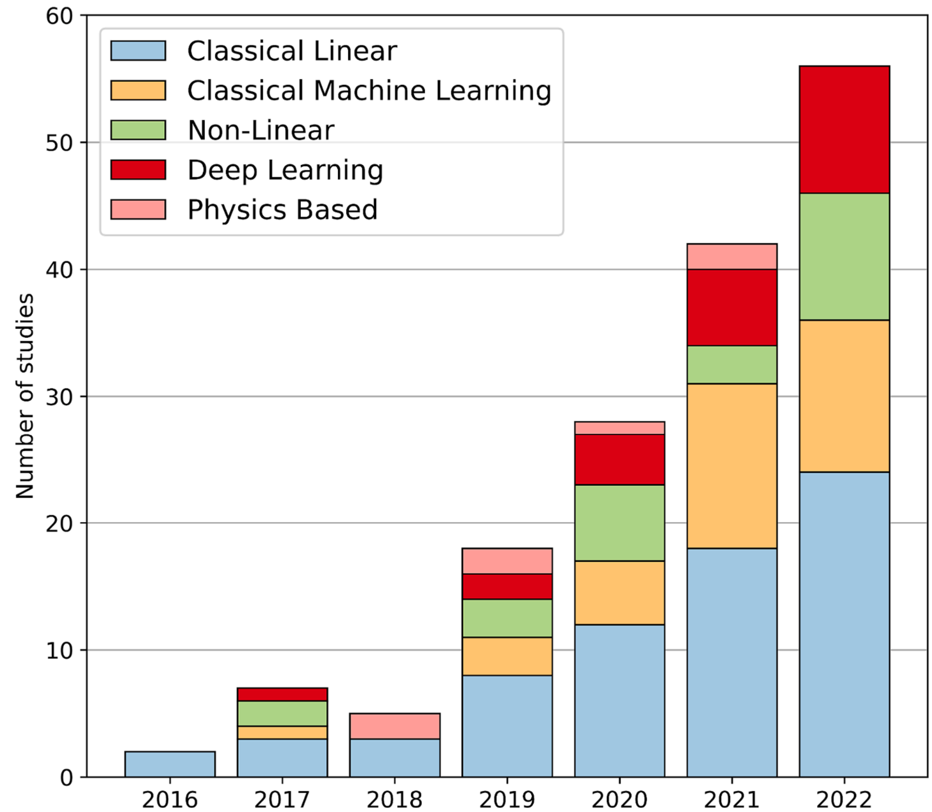

Fig. 5. Use of different model categories along the years used in the reviewed studies. Detailed information about the models included in each category can be found in the supplementary material (Supplementary Table S3). Vertical axis refers to the total number of studies using a given model. It may not coincide with the total number of papers, as some of them used different model types in their study.

concentration (>30 μg/L) (Shi et al., 2022). RF showed a good performance in several studies (i.e. Gómez et al., 2021). The hybrid machine learning model Binary Whale Optimization Algorithm (BWOA) was proven to perform well in a wide range of conditions having a great generalisation capacity and performing better than the traditional Artificial Neural Network (ANN) (Hassan et al., 2021), which might not be useful in the case of small lakes or when the sampling size is too small (Tian et al., 2022). Additionally, some deep learning models like GA–ANN showed better spatial transferability in comparison to the traditional Three-Band Model (TBM) (Chen et al., 2021).

The deep learning model showed an outperformance over all the other models in lakes, except over the physics-based model, and an outperformance over non-linear and physics-based models in coastal ecosystems (Table 3). Classical machine learning models performed significantly better than linear and non-linear models in lakes and better than non-linear and physics-based models in coastal ecosystems. Finally, physics-based models performed significantly better than linear and non-linear models in lakes. No significant performance difference between models could be established for reservoirs, rivers nor estuaries. It should be noted that the performance analysis done should be carefully interpreted, as model performance between different papers was compared even when they were applied using different indices and atmospheric correction models. The values of the whole set of goodness of fit parameters for all the model categories can be consulted in the Supplementary Table S11.

3.5. Water bodies in this review: Distribution and characterization

In terms of their geographical distribution, most studies were conducted in China, followed by Spain, USA and Brazil (Fig. 6), while Oceania and Africa were widely underrepresented, as well as some parts of Europe, Asia and South America.

Table 3
Model performance comparison through GLM results analysis. (<) and (>) represent the better or worse performance, respectively, of a comparison model in comparison to the reference model. (**) indicates a significant performance difference (p-value < 0.05) and (*) indicates marginal significance (p-value < 0.1). (n.s.) indicates no significant performance difference between AC models.

	Reference model	Sign and significance of comparison	Compared model
Lake	Classical linear	< **	Classical machine learning
		<**	Deep learning
		<**	Physics based
	Non-linear	< **	Classical machine learning
		<**	Deep learning
		<**	Physics based
	Classical machine learning	< **	Deep learning
Coast	Non-linear	< **	Classical machine learning
		<**	Deep learning
	Classical machine learning	> **	Physics based
	Deep learning	> **	Physics based

Regarding the type of studied ecosystem (Supplementary Figure S2), we found a bias towards studying lakes and reservoirs (37 % and 30 % of studies, respectively), while estuary systems were underrepresented

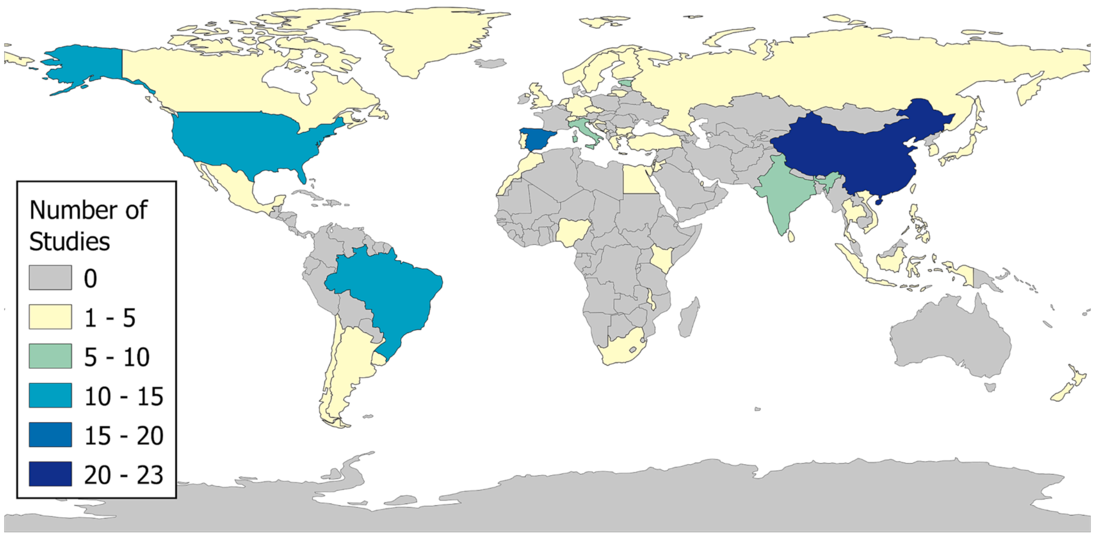

Fig. 6. Global uneven distribution of the number of studies indexed in Scopus and Web of Science that used Sentinel-2 satellite data to assess chlorophyll-*a* concentration in continental and coastal waters between 2015 and 2022. When a study included water bodies from several countries, it was counted in each country.

(both only 2 % of studies). Most studies just considered one ecosystem type. Three research articles studied several ecosystem types analysed separately, while seven studies included more than one type but combined all of them in the same database.

The studied water bodies ranged from 0.01 km^2 to 6,270 km^2, though many articles did not specify the area of their water bodies or just the minimum and maximum sizes. Despite 91 % of worldwide lakes being smaller than 0.025 km^2 (Downing and Duarte, 2006) and are relatively more threatened than larger water bodies, our results revealed that Sentinel-2 satellite data has not yet been widely used to monitor chlorophyll-*a* concentration in water bodies smaller than 1 km^2 (Fig. 7). On the contrary, water bodies ranging from 1 to 10,000 km^2 have been widely studied in the literature (40 % of studies), particularly between 10 and 10,000 km^2 (i.e. Z. Cao et al., 2022; Woo Kim et al., 2022), though such large systems account for a tiny percentage of the total number of water bodies worldwide (Downing and Duarte, 2006). This might be due to the limited spatial resolution of Sentinel-2 (10 m/pixel; Table 1) and also because the different methods tested in the literature and the existing pieces of software, such as SNAP, have shown to perform better in the biggest inland waters (Ansper and Alikas, 2019; Neves et al., 2021). Nonetheless, the spatial resolution of Sentinel-2 has been proven to be enough for the chlorophyll-*a* determination in inland water bodies (Hansen et al., 2017), including small inland lakes ranging from 0.05 to 3 km^2 (Toming et al., 2016).

3.6. Field sampling and measurement of chl-a concentration: Methodological aspects

A large majority of studies (89 %) used field data in combination with Sentinel-2 imagery but most of them omitted essential details on the field sampling methodology. A small percentage of studies that used field data detailed the time window between sampling and satellite overpass (46 % of studies), the depth at which the sample was collected (36 %), the distance to the shore (8 %), and none of them provided the depth of the water column at the sampling point. Most importantly, in the reviewed literature there was no defined methodology on how water samples for the chlorophyll-*a* determination were collected and on how these should be collected for successful remote sensing application

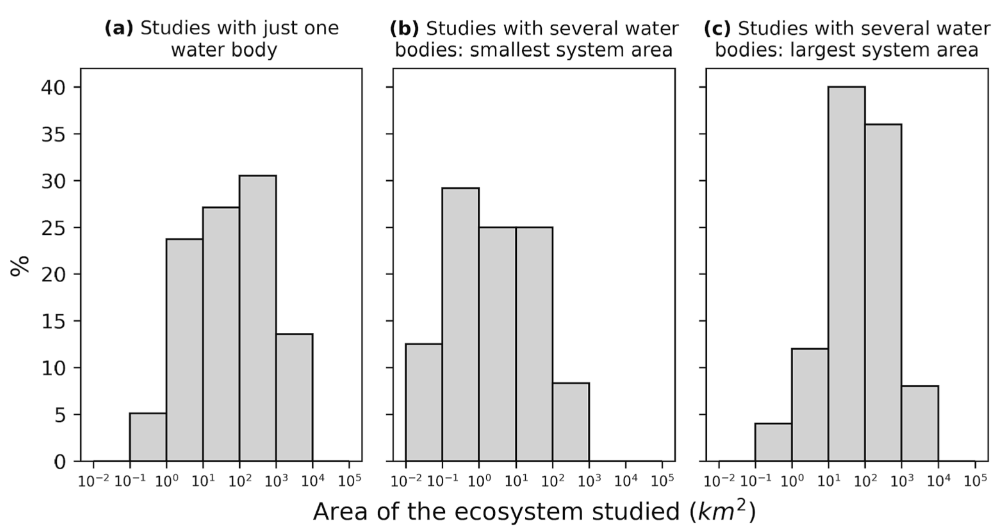

Fig. 7. Frequency intervals of the surface area range of the systems studied in the reviewed studies obtained from Scopus and Web of Science and that used Sentinel-2 satellite data to assess chlorophyll-*a* concentration in continental and coastal waters between 2015 and 2022. The horizontal axis is represented in a logarithmic scale. Studies analysing only one system are represented as single (a). In cases where more than one system was studied the minimum surface area of the smallest system (b) and the largest of the biggest (c) are represented.

purposes.

3.6.1. Time window between satellite overpass and field sampling

The time window, gap or span between the capture of the satellite image and the field sample, is an important parameter to take into account when comparing satellite imagery and field-sampling data. However, the effect of the time window in the chlorophyll-*a* retrieval has been the focus of a scarce number of the reviewed studies (46 % of the studies). Even so, the spatial, temporal resolution, and radiometric and spectral coverages of Sentinel-2 seem to allow lengthening the time window without impairment of the performance over satellites like Landsat 5 and 8, with which the maximal successful time span was of one and three days, respectively (Kayastha et al., 2022).

The temporal window was very variable in the different reviewed studies, ranging from hours (Ilteralp et al., 2022) to 12 days (Li et al., 2021). The longest temporal window that still showed a good performance seemed to depend on the system and on the season. For instance, in several Brazilian reservoirs, a 3-day time window performed as well as an exact same-day match (Aranha et al., 2022). In the case of artificial reservoirs, Kayastha et al. (2022) proved that using Sentinel-2 imagery the time window could be increased up to ±5 days (obtaining an R^2 of 0.71), although the best results were obtained when the time window was of up to one day (obtaining an R^2 of 0.84). However, a time span of one week between samples and image collection notably reduced this performance for chlorophyll-*a* retrieval and after one month the images were not valid even for the most stable parameters such as CDOM (Aranha et al., 2022). Hansen et al. (2017) found out that the suitable maximal time window was dynamic and depended on the season in eutrophic waters of Illinois, although a time window of ±2 days has been proposed to be ideal (Ambrose-Igho et al., 2021). In riverine ecosystems, which involve very dynamic processes, the maximal performance of the chlorophyll-*a* retrieval was achieved using a time window of ±3 h improving satellite-retrieved and in situ chlorophyll-*a* agreement by >30 % (Kuhn et al., 2019). Based on our review, the time gap between the capture of the satellite image and the field sample could be enlarged in cases where the system is more stable, the studied ecological processes are longer-term, and the water has a longer residence time. For instance, although it is beyond the scope of this review, in coastal areas, a time window of up to 10 days did not impair the performance of the used methodology (Ivanda et al., 2021).

3.6.2. Depth of the water sample

The depth at which the water sample was collected has been often overlooked in the studied literature, as only 36 % of the articles including field sampling methodology specified this parameter. This parameter greatly varied among the few articles that specified it, ranging from "surface samples" (without specifying the depth) (i.e. Soomets et al., 2020) to several discrete sampling depths along 100 m of the water column (Asim et al., 2021). Other studies, on the other hand, took integrated samples from the whole trophic layer (whole euphotic zone measured using the Secchi disk) (Bresciani et al., 2018).

Among the reviewed articles, the performance of the chlorophyll-*a* retrieval indices was not significantly affected by differences in sample collection depth since no significant statistical differences were obtained between them. Statistical differences were only obtained between non-specified sample collection depth and collection at a depth >0.5 m in reservoirs, a relationship from which no conclusion can be made. No other statistical significant result was obtained.

3.6.3. Distance from the shore

The distance from the shore at which the sample is taken is extremely important, especially in inland water bodies, in order to avoid or minimise the land adjacency effect. However, no specific studies on the topic were found through the search conducted in this review. Only 8 % of the reviewed papers specify this parameter in the methodology section, being mostly specified in small systems, where it would have the highest relevance. This scarce number of papers specifying this parameter did not allow to perform statistical analysis to assess this parameter. Warren et al. (2019) concluded that the adjacency effect affects the results when the distance from the shore is smaller than 0.5 km. However, Zhan et al. (2022) reduced this distance to 200 m in Mar Menor (SE Spain) to reduce the adjacency effect, whereas in (He et al., 2022) this distance was extended to 2 km. Nevertheless, this distance was reduced to 10 m in Zabaleta et al. (2021) where several lakes were compared because it was assumed that the effect of the adjacency effect would be similar in all of them, thus not affecting the results.

3.6.4. Total depth of the water column at the sampling point

No study specified the depth of the water column at the time and location of sampling. This might be a paramount parameter to consider during field sampling, as it will be crucial to avoid or minimise the bottom effect. Thus, knowing the specific bathymetry of the study area might be essential, as the bottom reflectance could have an influence on the satellite signal up to 25 m depth in clear waters (Marzano et al., 2021) affecting the results. Specially in systems that can be very shallow, such as rivers or very small and shallow lakes, the depth of the system at the sampling point is a paramount parameter to take into account to make sure that the signal received by the satellite comes from the plankton and thus avoid capturing chl-*a* signal coming from the benthos. However, only one out of the 11 revised articles working on rivers specified the depth of the system at the sampling time and the increasing level that the system experiments (Bhattacharjee et al., 2022).

3.6.5. Methodology for the measurement of chl-a concentration

The methodology used to obtain the ground truth for the chl-*a* concentration was diverse among the articles. The spectrophotometry methodology, including extraction both with acetone and ethanol (and quantifying or not the major degradation products of chl-*a*), and spectroradiometry were the most used (37.40 % and 11.45 % of the articles, respectively). 20.61 % of the articles did not detail the specific methodology used for that purpose. Several combinations of methodologies were used in 10.69 % of the articles, while fluorimetry and field multiparametric sondes were both used in 9.16 % of the reviewed articles. On the other hand, the HPLC (high performance liquid chromatography) was least used (1.53 % of the articles). Over time, spectrophotometry was always the most commonly used, while the use of multiparameter sondes increased drastically in 2022 (Fig. 8).

As stated before, the chl-*a* concentration varies greatly among different species and depending on the physiological state of the cells (Reynolds, 1984). This implies that the correlation between chl-*a* concentration and algal biomass may vary over time within the same study site. However, this might only cause an inaccurate estimation of the algal biomass but might not affect the field-satellite chl-*a* relationship. Moreover, other pigments as phycocyanin and phycoerythrin, which are present mainly in cyanobacteria, could affect the retrieval of chl-*a* due to overlapping absorption peaks at 620 and 560 nm (Viso-Vázquez et al., 2021), respectively. With the information available and being this discussion beyond the scope of this review, no methodology can be advised over others. This discussion is a large topic itself and has been widely discussed in articles, such as Wiltshire et al. (1998). A significantly better performance of fluorimetry over spectrophotometry was detected in lakes. However, this relationship turned out to be the opposite for reservoirs. Also in reservoirs, multiparameter sondes outperformed fluorimetry methodology. No other statistically significant result was obtained. The performance values of the different indices using different chl-*a* measurement methodology can be consulted in the Supplementary Table S12.

3.7. Other relevant methodological aspects

3.7.1. Spatial window around sampling points

Remote sensing analysis can be conducted using single-pixel or

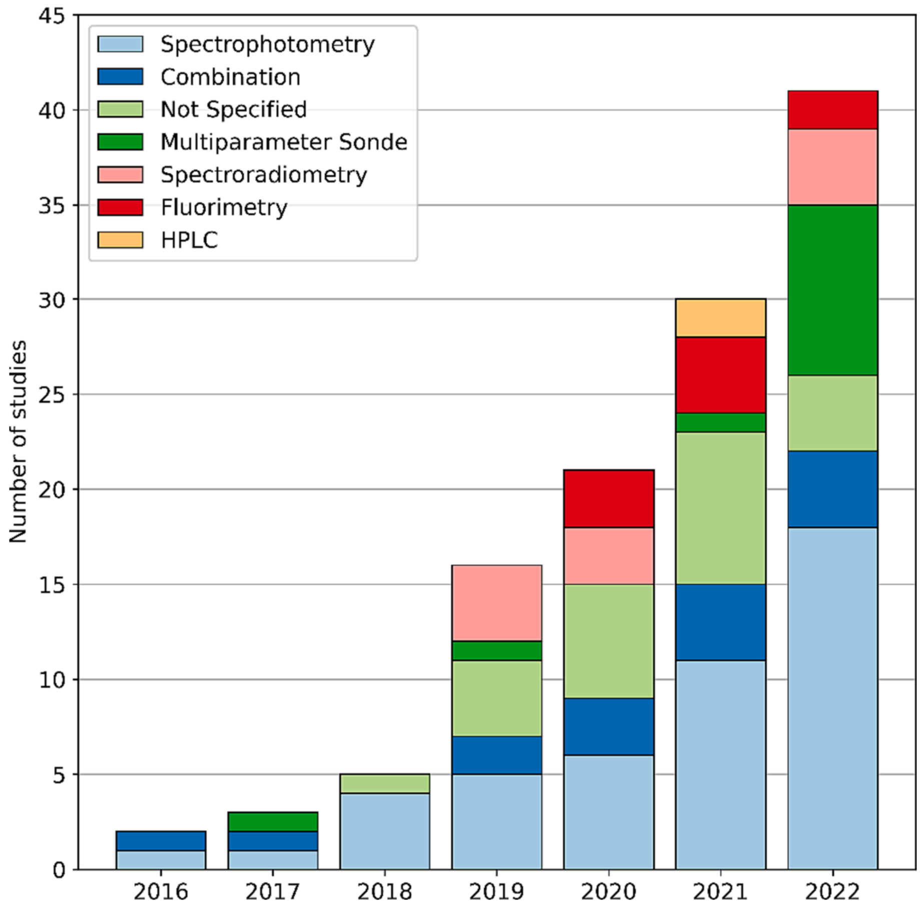

Fig. 8. Use of different chlorophyll-*a* measurement methodologies along the years used in the reviewed studies. Vertical axis refers to the total number of studies using a given model. It may not coincide with the total number of papers, as some of them used different model types in their study. HPLC: high performance liquid chromatography.

multiple-pixel analysis around the field-sampling pixel (i.e. 3x3 or 5x5 window size). The highest performance of the different models applied can be obtained from a different spatial window depending on the case (Ambrose-Igho et al., 2021). Li et al. (2022) determined that a 3x3-pixel spatial window was the best-performing in a Chinese reservoir. However, a balance should be found, as on the one hand, a bigger spatial window around the interest pixel provides a bigger context diminishing the potentially detrimental effect of outliers in the model performance. On the other hand, broadening this window could be counterproductive, as there is a major risk of heterogeneity among the pixels, not being representative of the field sampling point (Aptoula and Ariman, 2022).

3.7.2. Multisensor cross-band adjustment

Many indices were originally developed and validated for a specific satellite. Thus, when trying to apply it using a different one, homologue bands should be cross adjusted as was done by Ouma et al. (2020). Sentinel-2 has been seen to outperform other satellite sensors such as OLI (onboard L8) for the retrieval of chlorophyll-*a* concentration (Masoud, 2022). However, Ouma et al. (2020) found that OLI shows a higher signal-to-noise ratio in clear waters. A synergy between both sensors would increase the accuracy for frequent monitoring, as a combination of both sensors achieves a temporal resolution of 2–3 days which allows the temporal monitoring of systems with quicker dynamics than the individual temporal resolution of Sentinel-2 and L8 (Ouma et al., 2020). The fusion of a product with high spatial and low spectral resolution (S2) with a product with low spatial resolution and high spectral resolution (S3) might result in a fused product with enhanced both the high spatial and spectral resolution (Kremezi and Karathanassi, 2020). This combination has performed well in lakes for the detection of harmful algal blooms (Bresciani et al., 2020) and for the retrieval of different water quality parameters in lakes and reservoirs of the Mediterranean basin (Sòria-Perpinyà et al., 2021). The combined use of Sentinel-2 and MODIS has been seen to improve the performance of Sentinel-2 by limiting some of its restrictions, such as the adjacency effect (He et al., 2022).

Combining Sentinel-2 images with the ones from other satellites with a high spectral coverage might be beneficial as Sentinel-2 lacks a considerable range between band 9 (945 nm) and band 10 (1375 nm) and between bands 11 (1614 nm) and 12 (2202 nm) (Transon et al., 2018). Also, the lack of a spectral band at around 412 nm might limit the performance of chlorophyll-*a* inversion methods, as this band would improve the deconvolution of chlorophyll-*a* and other substances absorption.

Monitoring inland waters might require the combination of multiple sensors in order to benefit from the strengths of each one reducing the limitations and these should be selected according to the characteristics of the study area (Arias-Rodriguez et al., 2021).

3.7.3. Ancillary variables

The ability of empirical models to discern chlorophyll-*a* from covariant parameters such as total suspended matter is limited (Fernández-Tejedor et al., 2022). Also, the performance of band five (704 nm) might be lower in cases of high turbidity and abundant suspended matter (Xu et al., 2021). This is, however, beyond the scope of this review.

4. Lessons learned, knowledge gaps and ways forward

The rapid increase in the availability of remotely sensed imagery has driven a change in the perspective and opportunities for remote sensing monitoring of water bodies: (1) single or spaced sampling has been largely replaced by continuous and dense monitoring over time, (2) studies have evolved from single system or case studies to offer macroscale perspectives on trends in water bodies evolution, and (3) single-factor correlation analyses have been substituted by multivariate analyses and machine learning including auxiliary variables (Li et al., 2022).

Disturbingly, many reviewed studies did not include any ecological interpretation of their results nor at least an ecological description of the system but just pure mathematical relationships. A technical perspective alone in the pursuit of chl-*a* satellite monitoring may not be able to consider relevant ecosystem processes and patterns and could lead to ecologically misleading results. Indeed, the characteristics of the chosen satellite and image bands and the methods used to estimate water quality parameters must fit the underlying process dynamics of the study ecosystem. For instance, Perrone et al. (2021) found that the best performing model was different during stratification than during the mixing period in Italian lakes. Nevertheless, our review revealed a tendency towards an increase of studies that try to explain the satellite-observed changes in chlorophyll-*a* concentration from ecological variables and knowledge, particularly during 2022 (i.e. Woo Kim et al., 2022). Other parameters, which are greatly missing in the literature, are key to the chl-*a* concentration retrieval, such as the signal-to-noise ratio or the mixed pixel effect. Signal-to-noise ratio could not be considered as it was only taken into account in one of the articles analysed. The mixed pixel effect is related to the distance of data collection from the coast and the adjacency effect (discussed in section 3.6.3 of this review). It could not be discussed in detail because only 8 % indicated the distance to the shore and none of the revised articles discusses the possible presence of mixed pixels in their study.

Our review also revealed an essential need for satellite-based chlorophyll-*a* monitoring to specify (and ideally standardise) the chlorophyll-*a* field sampling protocol. Differences in sampling depth, distance from the shore, time window and other factors are seldom specified but could potentially pose a constraint in the model creation and further extrapolation to other systems or comparisons between models. These indications might be even more relevant in small and shallow water bodies where the adjacency and bottom effects are especially challenging.

In brief, the following recommendations for satellite-based monitoring of chlorophyll-*a* can be derived from our review, especially for lakes and reservoirs:

- The best and worst spectral indices to estimate chl-*a* were (see Supplementary Table S8 for full information):
- In lakes, the best performing indices were aphy(B4)/a*phy(B4), B7*(1/B4-1/B5), B5*(B6 + B4)/B2 and B3/B4, while the worst performing ones were (B1/B2-B2/B3)/(B1/B2 + B2/B3), (B1 + B2)/(B4/B2), B6*(1/B5-1/B4) and B8/B4
- In reservoirs, the best performing indices were B2 + B3 + B4 + B5, B3/B6 and (B5-B4)/(B5 + B4), while the worst performing ones were (B3-B2)/(B3 + B2) and B5-(B6 + B4)/2
- No significant differences among indices were observed in the rest of ecosystems (river, coastal and estuary).
- The best and worst atmospheric corrections to estimate chl-*a* were (see Table 3 for full information):
- In lakes, Sen2Cor and ATCOR outperformed ELM.
- In reservoirs, ATCOR performed better than the majority of the AC models, while C2XC AND Dark Object Subtraction performed worse than the majority of AC models.
- No significant differences among AC models could be observed in the rest of ecosystems (river, coastal and estuary).
- The best and worst chl-*a* satellite retrieval models were (see Table 3 for full information):
- In lakes, classical machine learning, deep learning and physics-based models outperformed linear and non-linear models, being deep learning models the best performing ones.
- In coastal ecosystems, classical machine learning and deep learning outperformed non-linear and physics-based models
- No significant differences among chl-*a* retrieval models were observed in the rest of ecosystems (estuary, river and estuary).
- No significant differences were observed among sampling depths.
- The best and worst field and laboratory techniques for chl-*a* measurements were:
- In lakes, fluorimetry performed better than spectrophotometry.
- In reservoirs, fluorimetry performed better than spectrophotometry and multiparameter sondes outperformed spectrophotometry.
- No significant differences among techniques for chl-*a* measurement were observed in the rest of ecosystems (river, coastal and estuary).
- The effect of the time window between field sampling and satellite overpass could not be statistically assessed due to the scarce number of papers specifying this parameter. However, from the discussions provided in the literature review, we could conclude that a time window of up to ± 2 h for rivers, ± 3–5 days for lakes and reservoirs and ± 10 days for coastal ecosystems would potentially perform well (see section 3.6.1 for more details).
- The effect of the distance from the shore at which the sample was taken could not be statistically assessed due to the scarce number of papers specifying this parameter (8 %). No recommendation can be made about this parameter since it was seldom discussed in the literature.

Despite remote sensing is a powerful tool for ecosystem monitoring, there are still important aspects to tackle in future studies to enhance chl-*a* retrieval from Sentinel-2 imagery in aquatic ecosystems:

- Detailed planning, design and description of the field and laboratory sampling methodologies (at least distance to shore, sampling depth, depth of the system at the sampling point, time lapse between the satellite overpass and the field sample, technique used to determine chl-*a* concentration) are key to assess and minimise undesired effects like shore adjacency, bottom influence, and system inertia on chl-*a* satellite estimates;
- Future studies should focus on systems smaller than 0.1 km^2 is, since they account for >90 % of the lakes in the world (Downing and Duarte, 2006) but still accumulate large challenges for the application of remote sensing techniques. The effect of distance to shore and depth of sample and water column must be particularly studied in these systems;
- A morphological and physical-chemical characterization of the water body and its basin might be needed as ancillary information to better estimate chl-*a*, as well as a reference for similar systems. In particular, collecting and reporting ancillary data such as TSS or CDOM is highly recommended since they affect the retrieval of chlorophyll-*a* concentration.

CRediT authorship contribution statement

Joana Llodrà-Llabrés: Writing – original draft, Conceptualization, Methodology, Formal analysis, Visualisation. **Javier Martínez-López:** Conceptualization, Formal analysis, Visualization, Writing – review & editing. **Thedmer Postma:** Formal analysis, Methodology, Visualization. **Carmen Pérez-Martínez:** Writing – review & editing, Conceptualization. **Domingo Alcaraz-Segura:** Writing – review & editing, Visualization, Conceptualization.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Joana Llodrà-Llabrés reports financial support and administrative support were provided by LifeWatch-2019-10-UGR-01. Carmen Pérez-Martínez reports financial support was provided by LifeWatch-2019-10-UGR-01. Javier Martínez-López reports financial support was provided by LifeWatch-2019-10-UGR-01. Thedmer Postma reports financial support was provided by LifeWatch-2019-10-UGR-01. Domingo Alcaraz-Segura reports financial support was provided by LifeWatch-2019-10-UGR-01.

Data availability

All data is available in the manuscript and in the supplementary material

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jag.2023.103605.

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