# SEMI-AUTOMATED PRODUCTION AND FILTERING OF SATELLITE DERIVED WATER QUALITY PARAMETERS

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**ABSTRACT:** This paper describes the semi-automated procedure implemented for the production of Water Quality Parameters (WQP) maps obtained processing Sentinel-3 and Landsat-8 imagery in the framework of SIMILE Interreg project. The processing chain includes the use of the C2RCC processor to obtain Chl-a (Chlorophyll-a) and TSM (Total Suspended Matter) and the Barsi method to produce maps of water surface temperature. The maps were filtered to exclude anomalous values due for example to clouds, water reflection (such as glint), or mixed pixels and compared to *in-situ* data. The filtering included an outlier rejection performed with the $3\sigma$ rule. The values singled out as local anomalies where checked with respect to possible local behaviours, such as the presence of very small gulfs and inflow/outflow streams and providing guidelines with visual examples, to support the operator. The idea of a procedure as much as possible automated and guided is to foster the WQP maps production after the end of SIMILE project.

## 1. INTRODUCTION

Remote sensing approaches have become a well-established practice for measuring inland Water Quality Parameters (WQPs) for decades (Topp et al., 2020). In recent years, the availability of open data, computational resources, and processing platforms, has encouraged the development and testing of algorithms to determine the water bodies constituents and their spatiotemporal modelling for addressing patterns (Topp et al., 2020). Now, remote sensing methods represent an opportunity for retrieving synoptic views of the water bodies to monitor the spatial and temporal variability of optically active WQPs (Giardino et al., 2014). A frequent and comprehensive monitoring of the quality of the aquatic ecosystems is crucial for the preservation of the water resource, and therefore to support the decision-making process of institutions watching for its conservation.

The study presented here is developed under the framework of the INTERREG Italy-Switzerland SIMILE project (Integrated monitoring system for knowledge, protection and valorisation of the subalpine lakes and their ecosystems), which focuses on the monitoring of the subalpine lakes of Como, Lugano and Maggiore in the Italy and Switzerland cross-border area with different techniques (Brovelli et al., 2019). This work concerns the satellite monitoring system implemented for the SIMILE project aimed at preserving the water quality of the subalpine lakes under study (Gerosa et al., 2021; Luciani et al., 2021). WQPs maps of Chlorophyll-a (Chl-a), Total Suspended Matter (TSM), and Lake Surface Water Temperature (LSWT) are produced using satellite imagery. Weekly Chl-a and TSM maps were obtained using the Sentinel-3 Ocean and Land Colour Instrument (OLCI), while monthly LSWT maps were produced using the Landsat-8 satellite Thermal Infrared Sensor (TIRS). This paper presents the semi-automated procedure set up for producing SIMILE WQPs maps, which includes satellite image processing and outlier rejection based on statistical filtering and the analysis of local conditions.

Because of human-driven nearshore activities and climate change, sustainable management of the quality of inland and coastal waterways has become a major requirement. Eutrophication, for example, which is mostly caused by growing agricultural and industrial activity, poses serious threats to ecosystem health, aquaculture and fisheries, recreation and tourism. In this context, geographically and temporally explicit data on water quality metrics are critical for improving our understanding of ecosystems and health, as well as assessing environmental impact of human pressure. In inland and coastal areas, field-based measurements of constituents have traditionally been an important source for monitoring water quality. *In-situ* observations, on the other hand, are constrained in both space and time, significantly limiting their utility for recording spatiotemporal dynamics of constituents like Chl-a, TSM, and CDOM (Coloured Dissolved Organic Matter). Furthermore, field sampling and laboratory analysis are both costly and time consuming. Remote sensing techniques are being investigated as a complement to in situ observations to address these difficulties. Every optically active component, such as Chl-a, TSM, and CDOM, affects the water-leaving radiance differently across the spectrum. Chl-a concentrations, or the photosynthetic pigment found in all phytoplankton species, are a common indicator of trophic status in aquatic environments. The dynamics of phytoplankton biomass, particularly harmful blooms, have an impact on the aquatic food web ecosystems, biogeochemical cycles and aquaculture. TSM stands for organic and mineral suspended solid solids in water, and it has a high correlation with turbidity and transparency of water (traditional measured with Secchi disk). Sediment transport, water quality evaluation and lake management research can all benefit from TSM's spatiotemporal monitoring. On land and in water, CDOM is a mixture of organic molecules generated by vegetation, algae, and bacteria. This property affects the quantity of light available in the water and can be used as a proxy for carbon concentration in lakes, which can aid carbon cycle research and water treatment efforts (Niroumand-Jadidi et al., 2021).

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## 2. WATER QUALITY PARAMTERS FROM REMOTE SENSING

Unlike *in-situ* data, remote sensing technologies can simultaneously monitor large areas with meaningful temporal coverage, capturing the geographical and temporal variability of optically active water quality parameters (WQP) (Giardino et al., 2014). Due to the general ongoing improvement of satellite sensor design and resolutions, inland water quality studies and monitoring applications based on optical satellites have increased dramatically in recent years (Bresciani et al., 2020; Topp et al., 2020). In addition to the normal point-based sampling procedures, Earth Observation has become a recognized and confirmed integrative strategy for monitoring lakes, allowing for a synoptic view of the water quality status.

Various compounds contribute to the optical signature of the water body, i.e. the concentration of the phytoplankton pigment Chlo-a, inorganic suspended sediments, and CDOM govern the light field reflected from the water surface of coastal waters, estuaries, rivers, and inland waters and recorded by an optical satellite (Brockmann et al., 2016). The retrieval of concentrations of these elements requires bio-optical models that contain the constituents' inherent optical properties (absorption and backscattering coefficients), concentration ranges and co-variations, and a mechanism for inverting the water leaving reflectance spectrum. Even though satellites measure the light field emerging from the top of the atmosphere, an atmospheric adjustment must be performed as part of the data processing for water. Because of the low reflectances on the ground, the atmospheric route radiance accounts for more than 90% of the signal seen by the satellite. As a result, atmospheric adjustment is critical (Brockmann et al., 2016).

For waters with CDOM, typical values of above-water remote sensing reflectance (Rrs) can be in the range of 1% in peak reflectance bands, and much lower in NIR areas with efficient absorption by water-soluble compounds. As a result, achieving a good signal-to-noise ratio is critical when inferring optical and biophysical properties of the observed water body from a remote sensor. In the visible spectrum, atmospheric path radiance surpasses water leaving radiance by at least 80%-90%, and this is primarily due to molecule and aerosol scattering in the atmosphere, which decreases with rising wavelengths (Warren et al., 2019). These signal components must be eliminated so that the residual signal may be assigned to the water's surface reflectance. Additional impacts at the water's surface, such as whitecaps, sun-glint, adjacency and proximity to land, may also be considered. These effects result in additional reflectance to that of the water column, posing problems for atmospheric correction. Validation of current procedures in a variety of water bodies and atmospheric circumstances is necessary to aid in the improvement of atmospheric correction routines (Gholizadeh et al., 2016).

For the spectrally based retrieval of constituents, a number of strategies have been developed, which can be divided into three categories (Niroumand-Jadidi et al., 2019): empirical methods, semi-empirical methods and physically based methods. This research follows the third strategy, which is a physically based approach that relies on inverting the radiative transfer model to obtain water body elements. The considered inversion technique is the Case 2 Regional Coast Colour (C2RCC) algorithm (Brockmann et al., 2016). The method entails utilizing neural networks that have been trained on a huge database of radiative transfer simulations.

Nevertheless, WQP map production relying on Remote Sensing products come with limitations and challenges that must be taken into account. The temporal resolution and number of WQPs produced maps are dependent on the weather conditions at the time of image acquisition: because SIMILE uses optical satellite images, it must deal with cloud covers that might obscure the sensors' view for days. When cloud covering did not cover the entire lake region, satellite images were processed. As a result, the dataset's temporal resolution is lower than the satellite sensors' revisit time (Hestir et al., 2015). Sun glint is a significant problem when observing water colour from space, resulting in anomalously bright pixels that should be treated (Overstreet & Legleiter, 2017). In addition, standard satellite data processing techniques, which are mainly designed for oceans, presume an unbounded water surface and, as a result, ignore the presence of neighbouring land. As an outcome, radiance reflected by the land and subsequently scattered by the atmosphere in the field of view of a satellite sensor observing the target water is a source of perturbations, resulting in water reflectance-based product errors. This phenomenon is known as adjacency effects, and it always happens when a scattering medium is placed in the proximity of a surface (De Keukelaere et al., 2018).

The optical characteristics of the lake waters under study, categorized as case 2 (to distinguish them from case 1 waters, corresponding to the oceans), are heavily influenced by inorganic and/or organic sediments, necessitating high accuracy in atmospheric correction methods to properly retrieve water parameters. The problem of atmospheric correction in case 2 waters has yet to be overcome. As a result, much effort has gone into developing atmospheric correction processors that span a wide range of methodologies (Warren et al., 2019, 2021). However, the performance of the processors varies depending on the scenario (sun and observation geometry, atmospheric, optical, and site-specific conditions), and there is currently no standardized approach; however, atmospheric correction processors continue to evolve as new methods and data become available. This brings the need to continue to test various atmospheric correction procedures as well as water quality retrieval methods using in situ data that accounts for a wide range of water types and environmental circumstances (Soriano-González et al., 2022; Spyrakos et al., 2018).

## 3. MAP PRODUCTION AND DATA FILTERING

### 3.1 Area of interest

In Italy, the geographical distribution of lakes is heavily skewed toward the Alpine and Subalpine areas. There are over 500 lakes with a surface area of more than 0.2 $km^2$ and a total volume of water of more than $150x10^9$ $m^3$ (Salmaso & Mosello, 2010). Around 80% of this water is concentrated in five lakes located along the Alpine chain's southern border, notably Lakes Garda, Iseo, Como, Lugano, and Maggiore (Deep southern Subalpine Lakes, DSL) (Salmaso & Mosello, 2010). Water is heavily used for hydroelectric power generation in the catchment areas of these lakes, whereas water is heavily used in agriculture and industry south of the DSL, in the plain of the River Po, becoming a life-sustaining element for the economy of Italy's most densely populated and productive area. Furthermore, these bodies of water play a significant role in the tourism business in the Alpine region. The DSL has drawn a great number of scientists from the beginning of limnological studies, promoting a large number of experiments in several sectors (Salmaso & Mosello, 2010), including local environmental agencies working on the conservation of these water resources. Thanks to the monitoring


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of these lakes, it was possible to examine some of the water quality parameters observed by the project with respect to reference data. In particular, ARPA Lombardia (Regional Environment Protection Agency, https://www.arpalombardia.it) field campaigns have been taken into account and CNR-IRSA (Italian National Research Counsil, Research Institute on Water) *in-situ* measures, collected also in the framework of CIPAIS, the international committee for the protection of Italy-Swizzerland waters (https://www.cipais.org/), devoted to the preservation of Lugano and Maggiore lakes. In addition, in the framework of SIMILE project, *in-situ* buoys/platform have been installed by ARPA Lombardia, CNR-IRSA and SUPSI (University of Applied Sciences and Arts of Southern Switzerland), partners of SIMILE, for high frequency monitoring of WQPs and time series of the acquired data are already available.

However, it is relevant to mention that the concentration of Chl-a can vary with depth and this can lead to inconsistencies among in-situ measures and values based on reflectance (Stramska & Stramski, 2005). The empirical water color algorithms for estimating the Chl-a are typically based on the correlation between the measured spectral reflectances, Rrs, and the measured surface Chl-a. This type of correlation does not count for the vertical structure of inherent optical properties. Two bodies of water with the same surface Chl-a but different vertical distributions of Chl-a(z) and associated inherent optical properties (IOPs) may have different values of Rrs(λ) at any wavelength. Therefore, the vertical distribution of Chl-a(z) may introduce errors into the algorithm-derived surface chlorophyll. By using an approach based on radiative transfer simulations it was shown that the percent difference in Rrs(λ) or in spectral ratios of Rrs(λ) between a vertically homogeneous water column (with the surface Chl-a identical to the homogeneous case) and a inhomogeneous water column can be significantly larger than 5% in many situations (Stramska & Stramski, 2005). With respect to our case of interest, *in-situ* measures, acquired with fluorimeters, are integrated in the 0-20m depth layer, while the remote sensing based maps take into account the first meters of water, depending on local conditions, mainly on water turbidity.

### 3.2 Image processing

SIMILE project uses satellite images to monitor the following primary WQPs (Brovelli et al., 2019) that are significant descriptors of water quality status on a regular and unrestricted basis: Chl-a and TSM concentration on the surface, and LSWT. The ESA Sentinel-3 A/B OLCI images have been used to map Chl-a and TSM concentrations since 2019, with a daily revisit period and a spatial resolution of 300m. LSWT was monitored using imagery from NASA Landsat 8's TIRS, which provided a spatial resolution of 100m with a 16-day revisit time. SIMILE also examines reported irregularities or unexpected concentrations in greater detail (10-20m) using ESA Sentinel-2 A and B MultiSpectral Instrument (MSI) images (Luciani et al., 2021). For SIMILE project, in between 2019 to 2021 the following WQPs maps have been produced: 283 for Chl-a, 283 for TSM and 109 for LSWT.

Images are processed using opensource and free technologies(Luciani et al., 2021), which have been validated for usage in inland aquatic environments (Free et al., 2021; Soomets et al., 2020), and are implemented in ESA's free software SNAP (Zuhlke et al., 2015). The Case 2 Regional Coast Colour C2RCC (Brockmann et al., 2016) employs a neural network to perform radiometric and atmospheric corrections as well as to compute Chl-a and TSM concentrations using Sentinel-3 data. Instead, LWST is calculated using the Barsi method (Barsi et al., 2005), methodology validated and used in different inland case studies (Sharaf et al., 2019; Amadori et al., 2021).

The C2RCC processor has proven to be suitable for inland WQPs mapping while defining the proper modelling parameters (Kyryliuk & Kratzer, 2019; Luciani et al., 2021; Toming et al., 2017). C2RCC processor for atmospheric correction has been updated: the current C2RCC is a modified version of the original Case 2 Regional Processor, which has been adapted to many multispectral satellites (e.g., Sentinel-2, Sentinel-3, Landsat-8). Now the C2RCC is composed by a set of three processors (i.e., C2-Nets: C2RCC, C2X, and C2X-COMPLEX) (Soriano-González et al., 2022).

The atmospheric correction performed by the C2RCC processor provided an accurate remote sensing reflectance (Rrs), as assessed in previous studies over the analysed water bodies (Luciani, 2021). It should be noted that the publicly available version of the C2RCC works only with the built-in atmospheric correction, which could be a limitation considering the sensitivity of the inversion to the quality of atmospheric correction, as discussed in the introduction. It should be considered as well the fact that for SIMILE project, there was the need to put in place a processing chain that could be as simple as possible in order to allow operators non-expert in remote sensing, such as offices taking care of the management of the lake, to perform the processing after the end of the project. For this reason, the open source SNAP software with C2RCC processor instead of scientific software such as, for example BOMBER (Giardino et al., 2012) or WASI (Gege, 2014) has been adopted.

The C2RCC neural net flags were exploited to automatically detect anomalies in the water spectra with respect to the training spectra and range (Rtosa_OOS, Rtosa_OOR Rhow_OOS: Rhow_OOR) and to detect the possible presence of clouds (Cloud_risk) (https://github.com/senbox-org/s3tbx/blob/master/s3tbx-c2rcc/src/main/java/org/esa/s3tbx/c2rcc/msi/C2rccMsiOperator.java). In case any of the flags were raised during the processing of the WQP maps, the disturbed pixels were excluded.

The WQPs maps production workflow described by (Luciani et al., 2021) has been automated in order to provide tools for ensuring the continuous production of the WQPs maps for the monitoring of the water resources by the public administration, even with limited expertise in remote sensing, after the end of SIMILE project. The image processing and filtering are implemented in a script that benefits from the SNAP-Python API (Zuhlke et al., 2015) to obtain the WQPs maps. The automated procedure for the computation of the WQPs eases the input of the different parameters and execution of the processing tools built-in SNAP depending on the workflow followed by a specific WQP. For example, for the estimates of Chl-a and TSM, the parameters required by the C2RCC processor to describe the water ecosystem (such as CHL factor, CHL exponent, TSM factor, TSM exponent, temperature, among others) are retrieved from datasets with time series for the parameters matching the date of acquisition of the Sentinel-3 imagery. In this case, the only variable parameter is the temperature retrieved periodically by ARPA Lombardia. While for the LSWT WQP maps, the procedure retrieves the parameters for Landsat-8 imagery at the date of acquisition for the atmospheric correction. The atmospheric correction parameters are the coefficient of atmospheric transmission, $\tau$, and the ascending/descending solar radiation, Lu/Ld, retrieved from (Barsi et al., 2005) (https://atmcorr.gsfc.nasa.gov/atm_corr.html), organized as time series in the working folder of the procedure.

The comparison with the *in-situ* measures provided by project partners as well as the inspection of the statistics of the WQP maps showed the need for the filtering of data to be marked as outliers and excluded from the maps. However, in the case of WQPs we are referring to values which could pertain to specific local behaviours, which implies that the filtering must avoid possible reasonable anomalies due to physical reasons. Thus, the time series of *in-situ* data have been considered, and the limnologists who study the waters of the lakes under study have been interviewed, in order to select the plausible ranges of values. To perform the outlier rejection, a 3σ filtering has been applied in order to single out data which showed a behaviour different from the one of the lake population. Then, the out-of-range values detected with the 3σ filtering were explored on the map to interpret the reason for the anomaly in terms of geographical location (e.g., lower surface temperature values could be reasonable when detected in an area affected by inflowing waters, higher surface temperature due to shallow waters, etc.) or image characteristics (e.g., lower temperatures due to cloud coverage). The goal of the entire filtering process was to remove pixels that could have resulted in a wrong measure while preserving as much information as possible.

In the following, some examples are shown, which are focused on Maggiore Lake. Figures 1 and 2 show the comparison among the Chl-a and temperature measures, respectively, observed *in-situ* by SIMILE buoy and the data obtained by SIMILE remote sensing based WQP maps before (orange) and after (grey) outlier rejection obtained with the 3σ rule.

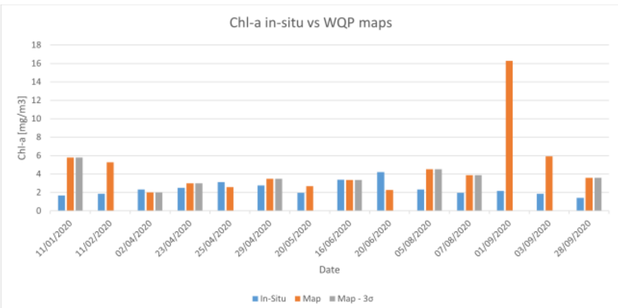



**Figure 1.** Comparison *in-situ* measurements and SIMILE remote sensing based Chl-a estimates, before (orange) and after (grey) outlier rejection

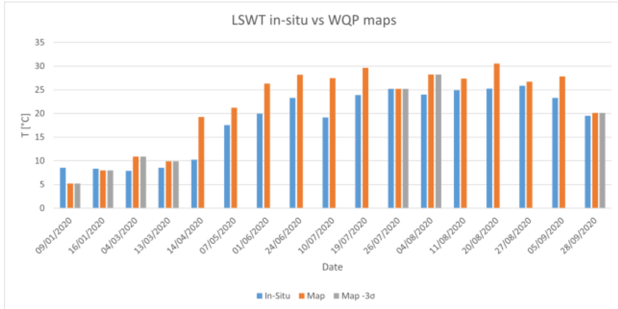



**Figure 2**. Comparison *in-situ* measurements and SIMILE temperature maps estimates, before (orange) and after (grey) outlier rejection

It can be observed that Figure 1 presents an evident outlier on the map produced for the 1st of September 2020, which disappears after the outlier rejection. This can be noticed also on Figure 3, which shows the Chl-a map before and after the filtering: the yellow pixel (zoom on the left), which corresponds to the SIMILE buoy, has actually a different behaviour with respect to the neighbouring pixels and it is filtered out after the outlier rejection. We can also observe that the buoy unfortunately is close to the lake shoreline, leading to possible issues related to mixed pixels between water and land.

Figure 2, as well, shows measures of temperature obtained from satellite-based maps before the outlier rejection (April to July) which are less in agreement with the local observations and which disappear after the 3σ filtering.

With respect to temperature, in some cases, the 3σ filtering caused the rejection of values that could be acceptable. For example, Figure 4 shows the Maggiore Lake bathymetry (on the right) and the LSWT SIMILE map before (top right) and after (bottom right) the 3σ outlier rejection for the map produced for 20th August 2020. It can be observed that the LSWT values have been filtered by the outlier rejection within the Angera gulf. However, the rejected values exceed of 1-2 °C the neighbouring unfiltered data and we can see that they correspond to very shallow water in a small gulf, which are conditions that could justify the increase in LSWT (Figure 5 shows the correlation between water depth and LSWT). For this reason, the procedure foresees the inspection of filtered data to prevent as much as possible the exclusion of acceptable values.

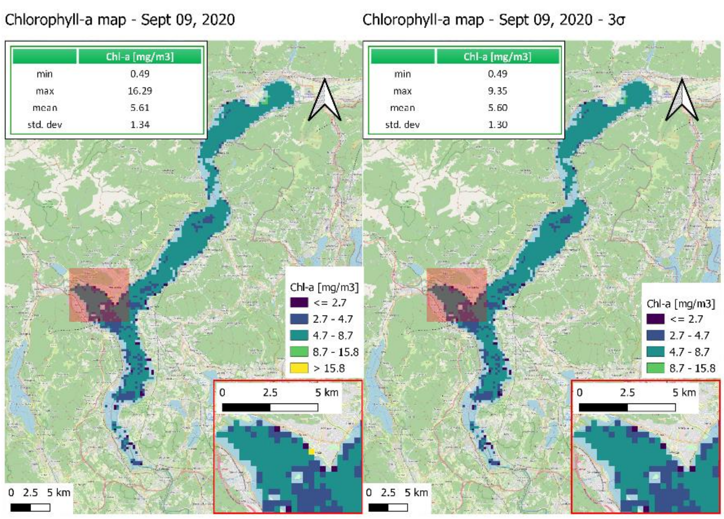



**Figure 3.** Pre- and Post- (left and right) outlier rejection using the three-sigma filter.

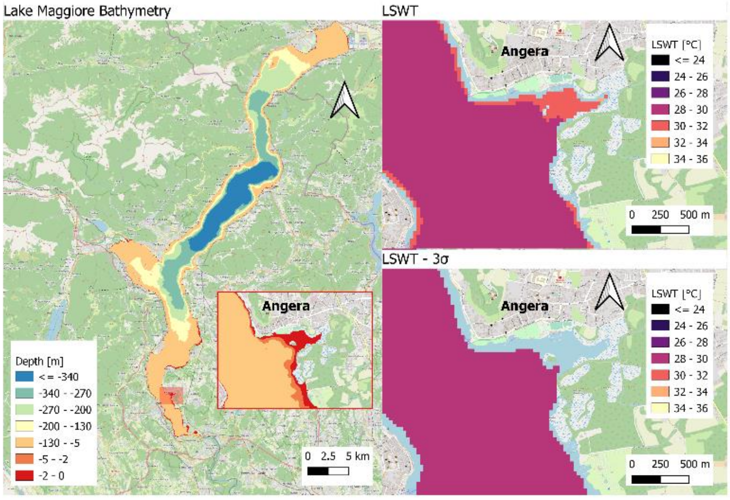



**Figure 4**. Maggiore lake bathymetry (on the left) and SIMILE WQP LSWT map of 20th August 2020 before (top right) and after (bottom right) the 3σ outlier rejection.

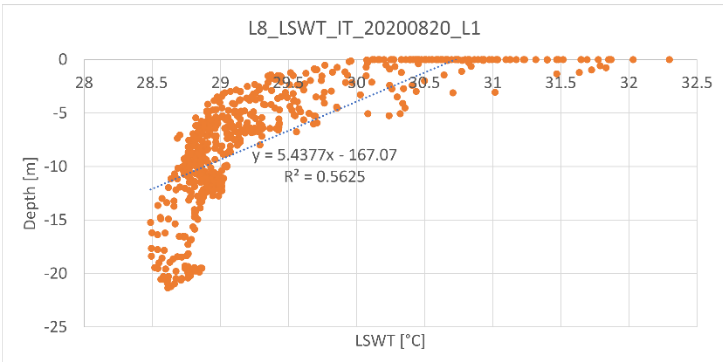
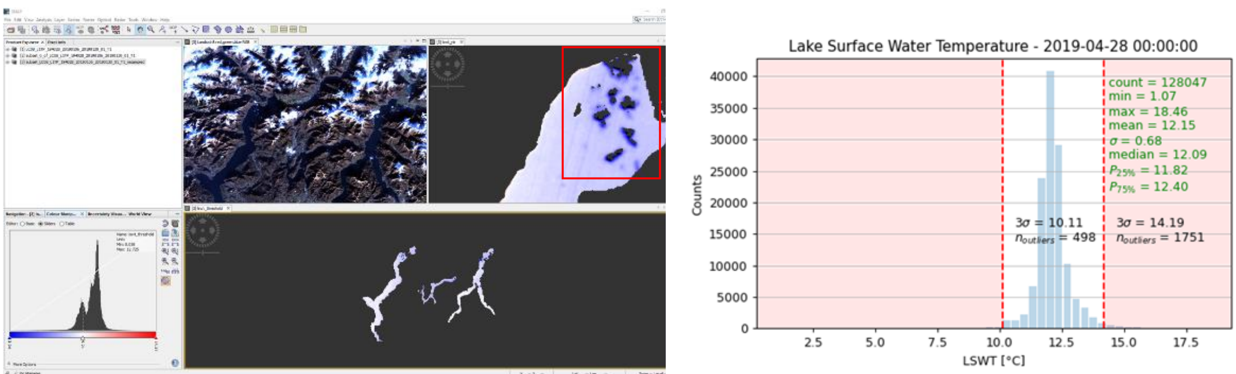



**Figure 5**. Correlation between water depth and LSWT for Maggiore lake in Angera gulf (see Figure 4)



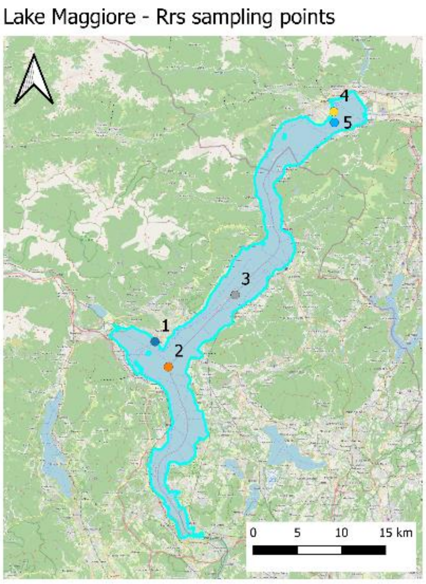

(a) (b)

**Figure 6.** Cloud coverage effects on LSWT WQP map. (a) Visual inspection in SNAP of LSWT anomalies of due to pixels surrounding cloud coverage. (b) Histogram and statistics of the LSWT map pixels

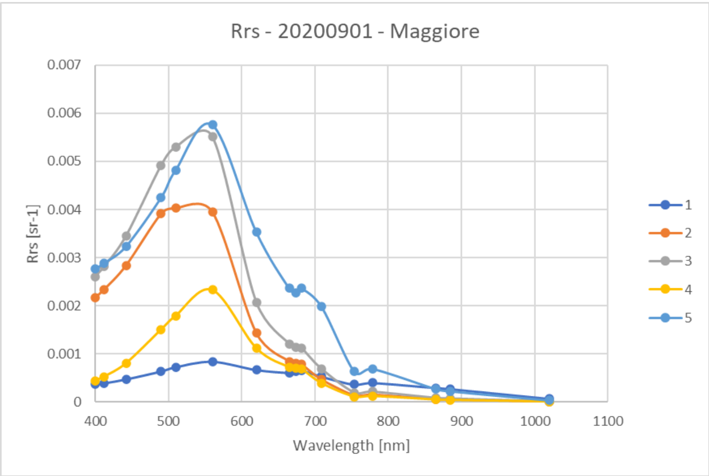
In other cases, the outlier rejection allowed to exclude additional pixels, with respect to the already filtered ones in SNAP and corresponding for example to very low values of LSWT, influenced by the presence of clouds (Figure 6).

In order to explore the reasons for anomalous values of Chl-a, a step back with respect to the output of the processor has been made, checking directly the reflectances. *In-situ* measures of reflectance, collected during dedicated field campaign with handheld WISP-3 spectroradiometers (Hommersom et al., 2012) have been taken into account and considered as reference. It was possible to single out the anomalous response (see Figure 7) of point number 1, which corresponds to the buoy position and to an outlier for the map produced upon the satellite image of 1st September 2020 (see also Figure 1).

To proceed exploring the direct analysis of the spectral signature to interpret anomalous values, a Principal Component analysis was performed on the reflectances of the image. It showed that the first eigenvalue was able to explain 95% of signal and it allowed to single out the outliers already detected by the processor flags, with some additional pixels that could as well be considered as outliers. This type of analysis, which is showing promising results, is still work in progress and will be further investigated.




(a)




(b)

**Figure 7**. Graph (b) shows the spectral signatures of the sampling points distributed on the lake (a), for the 1st of September 2020 Sentinel-3 image

## 4. CONCLUSION

In this paper, the processing chain and outlier rejection method applied for the production of satellite based WQPs maps, performed in the framework of SIMILE Italy-Switzerland Interreg project, is discussed. The map production has been designed using open source free software, such as SNAP, with the aim of automatizing and facilitating as much as possible the workflow to allow operators not expert in remote sensing to be able to perform the processing after the end of SIMILE project for lake water quality monitoring.

Local measures, provided by SIMILE project partners, have been considered as reference as well as in situ reflectance measures. Ancillary data have been taken in to account for complementing the metadata and support the analysis of the final WQPs maps such as: the sun light incidence to account for non-desirable effects in the processing such as glint, other adjacency effects due to the topographic configuration around the lake, visual examples of the previously mentioned disturbances to help the operator in the interpretation.

Outlier rejection has been applied to remove unacceptable values, trying to interpret, when possible, the reason for the anomalies in order to decide when the out-of-range values had to be included because due to peculiar conditions, such as high temperatures in small gulfs, or if they had to be discarded.

As further analysis, the spectral signatures rather than the final WQPs estimates are being considered to look for outliers. The principal component analysis is being exploited, to isolate disturbed pixels according to the spectral signature. The first results are encouraging, singling out the same outliers as the processors' flags with some useful addition. This will be investigated in the next future.

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