"FLEX 2018" CRUISE: AN OPPORTUNITY TO ASSESS PHYTOPLANKTON CHLOROPHYLL FLUORESCENCE RETRIEVAL AT DIFFERENT OBSERVATIVE SCALES

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Abstract – In frame of the European Space Agency's (ESA) "FLEXSense Campaign 2018" and the Copernicus Marine Environment Monitoring Service (CMEMS) project, the Global Ocean Satellite monitoring and marine ecosystem study group (GOS) of the Italian National Research Council (CNR) organized the oceanographic cruise "FLEX 2018". The CNR research vessel "Dallaporta" provided a ground station for several bio-optical instruments to investigate the coastal waters of the Tyrrhenian Sea (central Italy) in June 2018. The field measurements were performed in time synchrony with spaceborne (i.e. Sentinel 3A and Sentinel 3B satellites) and airborne (i.e. HyPlant airborne imaging spectrometer) observations, with the intent to contribute to calibration/validation activities for existing and future space mission developments. Particularly, active and passive fluorescence were investigated at different scales in aquatic ecosystems, to support preparatory activities of the FLuorescence EXplorer (FLEX) satellite mission to be launched in 2022. Results provide new insight on the sensitivity of Solar Induced Fluorescence (SIF) retrievals for atmospheric disturbances and other scale related aspects, and will eventually facilitate the implementation of robust retrieval schemes for the FLEX mission products. In addition, active fluorescence signals acquired from a LIDAR fluorosensor show a good agreement with SIF pattern retrieved by HyPlant and Sentinel-3 Ocean and Land Colour Instrument (OLCI). Our results demonstrate that the combination of active and passive fluorescence, together with the synergistic measurements from integrated platforms, is a promising approach to support the retrieval and interpretation of SIF in aquatic environments.

Introduction

Chlorophyll fluorescence is a fundamental proxy to provide physiological information and estimates of photosynthetic energy conversion efficiency. Long exploited in laboratory and field, the interest of the scientific community in remote sensing based fluorescence observations increased over the last years. Instruments adopting the Light Induced Fluorescence (LIF)

technique to remotely monitor actively stimulated fluorescence from dissolved and particulate sea water constituents have been widely employed for marine environment monitoring. [1]. In the recent years, large steps have been made also in the retrieval of passive Sun-Induced chlorophyll Fluorescence (SIF). In the framework of its Earth Observation Envelope Programme, the European Space Agency (ESA) is currently implementing the FLuorescence EXplorer (FLEX) satellite mission, the first mission specifically designed to monitor the photosynthetic activity of terrestrial vegetation. FLEX is scheduled to be launched in 2022 and comprises two spectrometers, the Fluorescence Imaging Spectrometer measuring in low (FLORIS-LR) and in high resolution (FLORIS-HR). Both sensors together cover the spectral range between 500 nm and 780 m and provide a varying spectral sampling interval and resolution of up to 0.1 nm and 0.3 nm respectively, particularly in the Oxygen absorption bands (O_2B and O_2A) [2]. Considering the complexity of the targeted photosynthetic process, FLEX will be ESAs first mission designed as "tandem concept", flying in tandem with the Copernicus Sentinel - 3 satellite. This allows measuring all relevant data to facilitate subsequent estimates of photosynthesis [2].

Measurement campaigns providing detailed in situ observations from integrated platforms at different scales play a crucial role to develop, calibrate and validate data products of current and future satellite missions [3]. In this context, ESA organized the "FLEXSense campaign" in 2018 to facilitate preparatory activities for FLEX, particularly addressing the development of retrieval schemes and atmospheric correction approaches. The campaign specifically focused on the collection of hyperspectral data over monitoring sites in vegetation ecosystems such as agricultural and forest sites, and aimed to evaluate the potential applicability of FLEX data to assess coastal marine environments.

SIF retrieval in aquatic ecosystems has a great ecological value considering its potential in discriminating phytoplankton diversity and in improving productivity estimates. Particularly, in optically complex waters, characterized by active constituents with very different dynamics compared to open waters, the retrieval of SIF is a major challenge. McKee et al. [4] explored coastal waters with CDOM and TSM ranging from 0 m^{-1} to 1 m^{-1} and from 0 g m^{-3} to 10 g m^{-3} respectively, and found that increasing concentrations of CDOM and minerals can reduce the water-leaving SIF per unit chlorophyll by over 50 %. This suggests caution in the interpretation of SIF signals from coastal waters [4] and highlights the crucial role of the in-situ bio-optical characterizations for SIF retrievals and validation activities in aquatic ecosystems in general and coastal waters in particular. In this context, CNR-ISMAR organized in frame of the FLEXsense campaign the oceanographic cruise "FLEX 2018". The CNR research vessel "Dallaporta" provided a ground station for several bio-optical instruments that investigated the coastal waters of the Tyrrhenian Sea (central Italy) in June 2018. All the Apparent and Inherent Optical Properties (AOPs and IOPs) were estimated in addition to various physical ancillary data. These detailed in-situ measurements were complemented with concurrent radiometric observations acquired using the high-resolution airborne imaging spectrometer HyPlant [5] and both Sentinel - 3A and - 3B satellites.

The aim of this work is to assess whether SIF can be consistently retrieved using a simple retrieval scheme for in-situ, airborne and spaceborne measurements and if, in the framework of this integrated approach, TChla active fluorescence, less affected at 680 nm by other constituents, can be useful to improve the retrieval of passive fluorescence and the understanding of its behavior.

Materials and Methods

The "FLEX 2018" cruise took place between 5th and 7th of June 2018 in the Tyrrenian Sea. Figure 1 shows the sampling plan of the cruise in the investigated area. The sampling strategy was optimized to facilitate the objectives of the "FLEXSense Campaign".
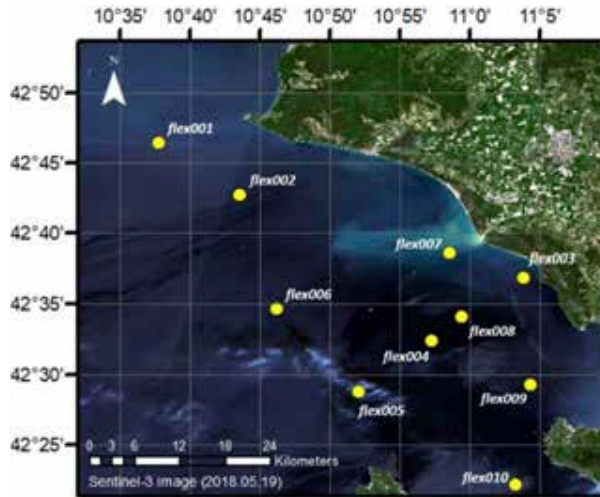

Figure 1 - FLEX 2018 in-situ sampling plan. Yellow circles indicate stations intensively characterized by in situ sensors. The background true color image was obtained by Sentinel-3.

For each measurement station, in-situ data for the determination of CDOM, algal and non-algal absorption coefficients (a_{CDOM}, a_{phy} and a_{NAP} respectively) and phytoplankton pigments and Total Suspended Matter (TSM) concentration were collected at the surface. Water was sampled by a horizontal hand Van Dorn bottle. For all parameters except CDOM, water was pre-filtered by a net with a mesh of 250 μm to eliminate the zooplankton component and different water volumes, dependent on the optical properties, were vacuum filtered through Whatmann GF/F glass microfiber filter (nominal porosity 0.7 μm). Samples for particle absorption and pigment concentration were stored in liquid nitrogen, while those for TSM were stored at -20 °C. CDOM filtrations were carried out by low pressure through 0.2 μm Nylon filters. Filtered water was stored in black Pyrex bottles at -4 °C until measurements have been performed in laboratory. With regard to the instruments and analysis methods, pigment concentrations were estimated by High Performance Liquid Chromatography (HPLC, Agilent 1260) implementing the method of [6]. The absorption measurements were carried out by a dual beam Lambda 19 Spectrophotometer (Perkin-Elmer), equipped with a 50 mm integrative sphere for the particulate only. Methods of [7] and [8] were adapted for estimates of dissolved and particulate material absorption respectively. The analysis of TSM concentration were carried out by a gravimetric method following the protocol of [9].

Continuous LIF measurements were carried out using a LIDAR fluorosensor system developed by the ENEA agency in collaboration with the INSIS company in frame of the Italian Regional Project "RIMA" and installed on the ship. The light source is a frequency-tripled Nd:YAG laser (355 nm) and the detection system combines a telescope, wavelength dependent beam splitters, interference filters and Avalanche PhotoDiodes (APDs) being more compact and robust than photomultiplier tubes. LIF data are corrected with respect to the solar background and normalized to the Raman signal collected at 405 nm (Raman Unit, R. U), making it insensitive to instrumental variations [1]. The fluorescence signal has also been calibrated as TChla and compared with TChla data obtained from VIIRS (Visible Infrared Imaging Radiometer Suite) on 8th June, the first satellite data available due to cloud cover on campaign days and retrieved by applying the regional MedOC4 algorithm [10].

Above water surface radiometric measurements were collected in 8 of the 10 stations sampled using the in-situ fluorescence spectrometer FLOX (jb-hyperspectral.com). Sampling activities took place in concurrence with HyPlant and Sentinel-3 scene acquisitions. The spectral characteristics of the three systems in terms of sampling interval and resolution are comparable (cf. jb-hyperspectral.com, [2], [5]). FLOX comprises two sensors to measure irradiance and radiance in high and low spectral resolution, comparable to HyPlant and FLEX sampling schemes, making this instrument a good candidate for the multi-scale assessment of SIF retrieval accuracy in coastal areas. However, the instrument needs to be reconfigured to facilitate the simultaneous acquisition of downwelling irradiance (E_d), upwelling radiance (L_u) and sky radiance (L_{sky}), the three quantities required by specific protocols for spectroradiometric observation in aquatic systems.

HyPlant data were acquired over a coastal area near the Ombrone River in a North-South oriented flight path up to roughly 20 km from the coastline on 6th of June. The original HyPlant spatial resolution (3 m) was resampled to 300 m to facilitate the comparison with Sentinel-3 data. Since Sentinel-3B data acquired during the cruise day was substantially cloud covered, we used Sentinel-3 L1A data from 10th of June 2018 instead.

SIF was retrieved from in-situ, airborne and spaceborne measurements in SNAP using the Fluorescence Line Height (FLH) algorithm, an established empirical algorithm that exploits radiances at and around the SIF emission in three spectral bands (for this work 665 nm, 681 nm and 709 nm). For more details on the algorithm approach, its general formula and the selected spectral bands see [11], [12], [13]. The FLH method is typically used in the open ocean since low signal from elastic scattering provides good resulting baseline curves [14], [15] . High TChla and TSM concentrations in optically complex waters could significantly affect FLH results due to a peak from the elastic reflectance overlapping with the fluorescence signal and therefore potentially contaminating fluorescence retrieval [11].

Results

The compositional variability of the IOPs in each station is shown in Figure **2** using ternary plots, which feature a_{CDOM}, a_{phy} and a_{NAP} at four characteristic wavelengths, 443 nm, 560 nm, 620 nm and 680 nm [16].
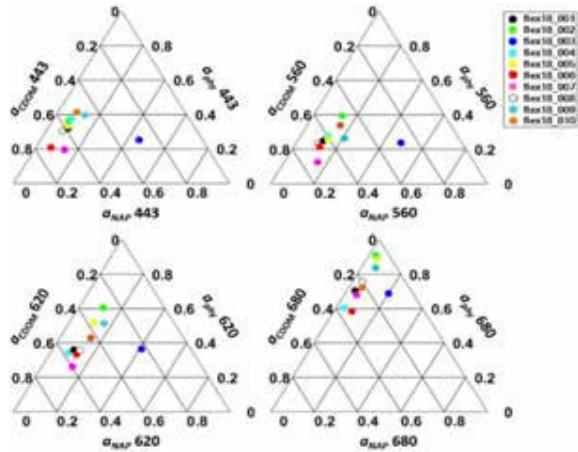
Figure 2 - Ternary plot showing the compositional variability of the IOPs in each station.

At 443 nm, where all three components absorb significantly, data show that in general the absorption budget is dominated by CDOM. Low values of a_{NAP} were found also at 560 nm (band usually governed by NAP absorption), except for station 3. The ternary plots at 620 nm and 680 nm indicate stations 2, 5 and 9 as the most characterized by phytoplankton absorption, also in terms of phycocyanin absorption (typical at 620 nm and proxy for cyanobacteria). All over the cruise, TChla and TSM concentrations range from 0.08 mg m^{-3} to 0.31 mg m^{-3} and from 0.13 g m^{-3} to 1.65 g m^{-3}, respectively. The relations between TChla and TSM and a_{CDOM} highlighted a more coastal feature for stations 3 and 7 (data not shown).

The relation between TChla concentration derived from HPLC measurements and FLH based – SIF values derived from FLOX (performed in 8 of the 10 stations) is shown in Figure 3 (left panel). On the right panel in Figure **3**, the same relation but using LIF data detected from LIDAR in-situ acquisition is illustrated.
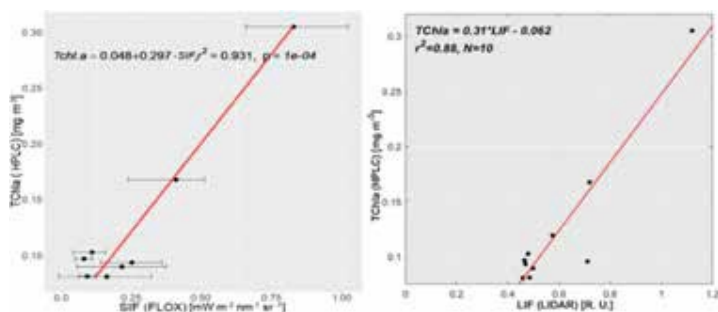

Figure 3 - In-situ estimates of TChl-a vs SIF (FLOX) and LIF (LIDAR).

For both in-situ instruments, derived fluorescence and TChla concentrations show a good agreement (i.e. $r^2 = 0.93$ and 0.88, respectively). It must be noted that the correlation for the LIDAR is slightly lower due to the TChla value in station 10, while no FLOX measurements are available for this station.

FLH based SIF retrieved from HyPlant and Sentinel-3 data is show in Figure 4.

When comparing the SIF data obtained from airborne and spaceborne in the corresponding swath, similar spatial patterns can be observed. Figure 5 (left panel) shows a comparison of SIF dynamics obtained from both sensors along a coast to offshore transect (black line in Figure 4). However, the range of SIF values calculated from HyPlant and Sentinel-3 differs significantly. In particular, SIF derived from Sentinel-3 FLH processing resulted in numerous negative values.

The spatial SIF pattern of from HyPlant and Sentinel-3 OLCI along the coast to offshore transect was also compared with the LIF signal (Figure 5, right panel), using the data overlapping with the airborne track (Figure 6, left). LIF signal shows a behavior comparable
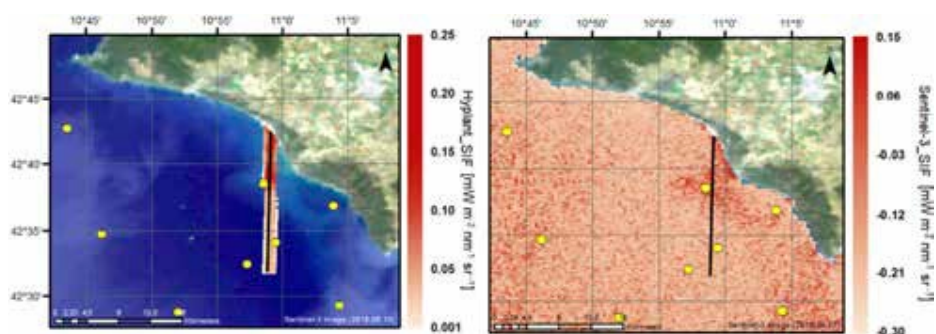

Figure 4 - SIF values calculated for the study area from HyPlant (left) and Sentinel-3A (right). The black N-S line indicates a transect used in Figure 5 (left panel).
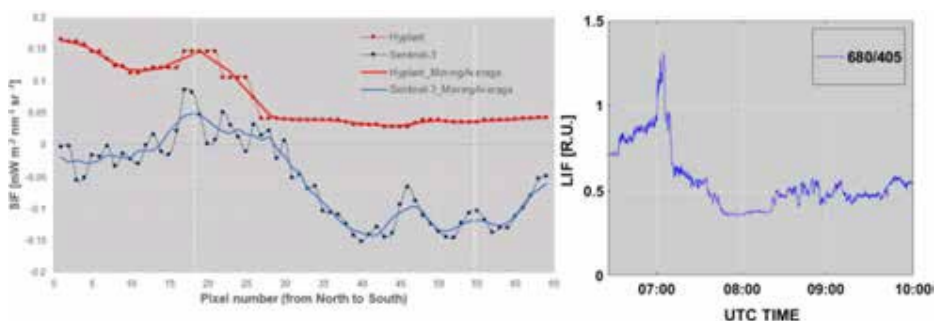

Figure 5 - SIF from HyPlant and Sentinel-3 OLCI from coast to offshore (dashed line with points) and smoothened profiles using a moving average approach. White dotted lines enclosed the pixels where HyPlant and LIDAR acquisition overlap (left). The corresponding LIF signal is shown to the right.

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with the SIF obtained from the other two sensors, with increasing values in proximity of station 7 closer to the coast that gradually decrease and then stabilizes offshore. In the right panel of Figure 6, the LIDAR data collected during the whole cruise and calibrated in TChla is shown with respect to VIIRS TChla data.
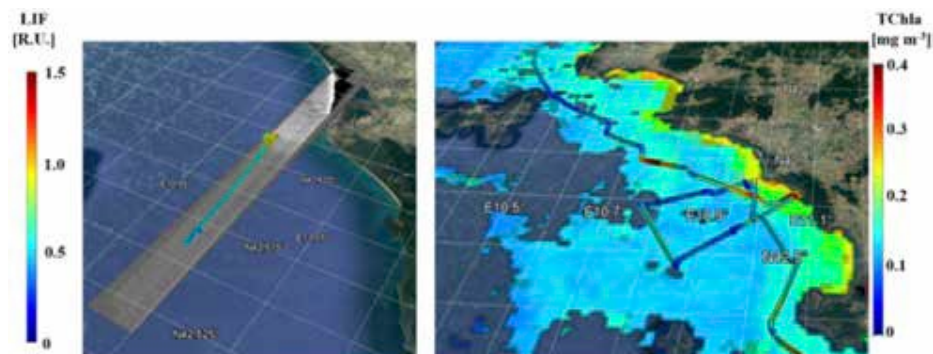

Figure 6 - On the left, LIDAR LIF data overlapping the HyPlant track and used in Figure 5. On the right, LIDAR data acquired over the all cruise (05 – 07 June) calibrated in TChla concentration and shown with respect to VIIRS TChla data related to the 8th of June.

Discussion

Based on the relative contribution of the three active constituents (i.e. phytoplankton, yellow substances, suspended material) to the total absorption, all investigated stations can be classified as complex waters dominated by yellow substances [17], except station 3 that is dominated by NAP. The ranges found for TChla and TSM concentrations and a_{CDOM}, suggest that the SIF retrieval based on the FLH approach could yield good results in this type of water. The evaluation of in situ SIF and LIF with TChla measurements (Figure 3) indicates a good positive correlation between both quantities. This finding corresponds with the known fact that higher phytoplankton biomass leads to higher fluorescence emissions. However, we only had a few sampling locations with most points dominated by low TChla concentrations and the linear regression is mainly driven by two points with higher fluorescence and TChla values. Future analysis would require more measurements and a sampling following gradients of chlorophyll concentrations, preferably closer to the shoreline, to properly account for the heterogeneity in this dynamic region. Further, only the upwelling radiance measurements from the FLOX were used for the FLH based SIF retrieval. It would be important to assess the impact of this configuration on the SIF-retrieval and advantageous to improve the FLOX design to facilitate standard aquatic measurement protocols.

SIF values derived from FLOX and HyPlant have similar magnitudes and trends but the SIF maximum from FLOX is four times that from HyPlant. This divergence can be possibly, among other effects, attributed to a missing atmospheric correction of HyPlant data. We also observe comparable spatial pattern between the airborne and spaceborne based SIF retrievals, with a coast to offshore gradient (Figure 4 and Figure 5, left). The same gradient

is also evident in the LIF data (Figure 5, right and Figure 6, left). This expected behavior is caused by the gradient in biomass that decreases with the distance from the coast. This is also confirmed by the TChla values found in the two sampling stations that fall into the HyPlant acquisition area, station 7 (more coastal) and 8. SIF and LIF values were also affected by the discharge coming from Ombrone River, which coincides with the higher FLOX based SIF values calculated especially near the river delta and the peak in SIF and LIF values between 15-25 pixels in Figure 5. The influx of additional constituents, particularly of algae and nutrients, contributes to an increased biomass concentration and thus a higher SIF and LIF signal in coastal waters surrounding the river outflow and in correspondence with station 3, the most coastal station, where the highest in-situ SIF and LIF values and TChla concentrations were obtained. Despite the common spatial pattern, however, the range of SIF values calculated from HyPlant and Sentinel-3 data substantially differ (Figure 5). The numerous negative values from Sentinel-3 FLH retrieval is likely due to the relatively low TChla concentrations in the study area. Perhaps the main reason for the difference in HyPlant and Sentinel-3 SIF results is the detection limit of Sentinel-3 OLCI due to its SNR combined with unfavourable atmospheric conditions. A similar study [18], using FLH in oligotrophic waters, showed good results for field data set but negative values from MERIS. The authors attributed this result to MERIS detection limited which appears to also be applicable for Sentinel-3 OLCI in this case. It must be noted that we did not account for effects of optically shallow waters, adjacency effects and stray light in our calculations, which could also affect the results obtained.

Conclusion

We conclude that the FLH approach is effective in measuring SIF in our study area, but further investigations to assess the general suitability of this method for different water types is important, e.g. by extending our approach to a wider range of optically complex waters that are typical of coastal regions. Particularly, at higher TChl-a concentrations (5 mg m^{-3} to 7 mg m^{-3} [4], [19]) and TSM concentrations, the apparent SIF peak observed at 685 nm appears to "shift" to a longer wavelength due to overlapping of SIF emission region and strong elastic scattering in the NIR [20]. Since such elevated concentrations are common in coastal and inland waters, especially during algal bloom events in spring and summer, refinements of the standard FLH approach are possibly needed to avoid a violation of method inherent assumptions. We suggest to consider more sophisticated retrieval schemes based on high spectral resolution data to possibly define more robust strategies to disentangle SIF from non-SIF signals.

Our results indicate that consistent SIF retrievals from in situ to airborne and satellite platforms are possible in relative terms and obtained spatial pattern are expected for coastal areas [21], [22]. Absolute differences in retrieved SIF across scales, however, require further investigations. Our approach allows to set priorities for the refinement of further pre-processing (e.g. implementation of more sophisticated atmospheric correction schemes) and to understand possible future limitations of retrieving SIF due to SNR.

The good agreement between active LIF signals from LIDAR fluorosensor and passive SIF values retrieved from FLOX, HyPlant and Sentinel-3, demonstrates how the connection between active and passive fluorescence, combined with measurements from integrated platforms, can be a promising approach supporting the development and evaluation of SIF retrieval approaches and contributing to phytoplankton fluorescence interpretation.

Acknowledgments

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