

CONNECT (SO287) Oceanographic Campaign - RV SONNE Data Processing Report Underway chlorophyll-a and turbidity

Abstract

This report describes the processing procedures of underway chlorophyll-a and turbidity data acquired during the SO287-CONNECT cruise on board the German Research Vessel *SONNE*, including scientific visualization and tabulation of the datasets. The SO287-CONNECT oceanographic campaign aimed to cross the North Atlantic Ocean from Las Palmas (Gran Canaria, Spain) to Guayaquil (Ecuador, in the Equatorial Pacific Ocean) between 11 December 2021 and 11 January 2022.

Authors:

Alexandra Rosa, Cláudio Cardoso, Jesus Reis, Cátia Azevedo, Rui Caldeira, André El-Ama*, Daniela Voß*, Rüdiger Röttgers**, Helmke Hepach***, Birgit Quack***

*ICBM, Deutsche Allianz für Meeresforschung (DAM)

**Helmholtz-Zentrum Hereon

***GEOMAR Helmholtz Centre for Ocean Research Kiel

Contact:

email: alexandra.rosa@oom.arditi.pt; rui.caldeira@oom.arditi.pt

January 2023

Index

1. Introduction	1
2. Data acquisition, processing and calibration procedures	1

1. Introduction

The SO287-CONNECT oceanographic campaign aimed to cross the North Atlantic Ocean from Las Palmas (Gran Canaria, Spain) to Guayaquil (Ecuador, in the Equatorial Pacific Ocean), passing by the Sargasso and Caribbean Seas, during four weeks on board the German Research Vessel *SONNE* (between 11 December 2021 and 11 January 2022). Underway measurements of chlorophyll-a and turbidity were performed along the cruise transect. In this report, we describe the processing procedures applied to these datasets, including calibration procedures.

2. Data acquisition, processing and calibration procedures

The underway data were performed using two independent Self-cleaning Monitoring Boxes (SMB_A and SMB_B). The SMB measured the following variables: sound velocity (AML MicroX SV), internal temperature and conductivity (SBE 45 thermosalinograph), and fluorescence (chlorophyll-a) and turbidity (Wetlabs FLNTU). Salinity was further calculated based on the internal temperature and conductivity measurements. In addition, external temperature measurements were performed at two water inlets at ~4 m depth (SBE 38). The two systems recorded alternately along 14 hours, of which the systems recorded data simultaneously for around 2 hours at each transition. While one was measuring, the other one was in cleaning mode. For further details about the equipment specifications, please refer to the handbook of the RV *SONNE*¹.

Data were downloaded from the DSHIP database at one-second resolution (data files named as SMB_A_clean.csv and SMB_B_clean.csv). For the processed temperature and conductivity/salinity datasets, please access to the OSIS portal² and PANGAEA Data Publisher³. Figures 1 and 2 show the chlorophyll-a and turbidity raw data acquired by SMB_A and SMB_B, respectively. It is important to note that a malfunction of the fluorescence sensor (SMB_B) occurred between 15/12/2021 and 22/12/2021 (identified by a red box in Figure 2), resulting in sometimes negative values. This sensor was then replaced by a new sensor of the same model.

¹ <https://www.lfd.uni-hamburg.de/en/sonne/technisches.html>

² https://portal.geomar.de/kdmi#_48_INSTANCE_5P8d_=_metadata%2Fleg%2Fshow%2F359749

³ <https://doi.pangaea.de/10.1594/PANGAEA.953082>

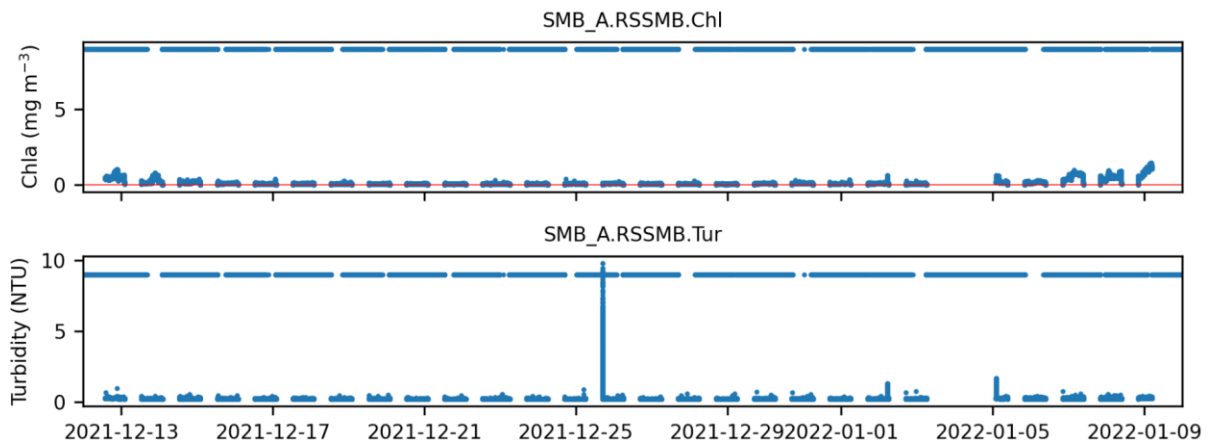


Figure 1 - Time series of chlorophyll-a concentrations, and turbidity acquired by the SMB_A (raw data).

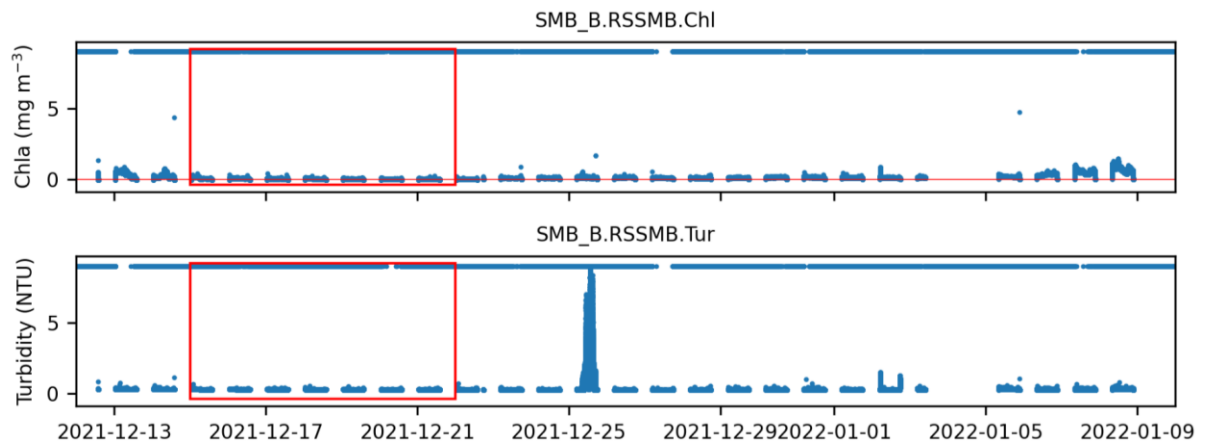


Figure 2 - Time series of chlorophyll-a concentrations, and turbidity acquired by the SMB_B (raw data). Red boxes represent the period of malfunction of the fluorescence sensor.

Data processing procedures consisted on six main steps: i) dummy values (i.e. 9) were replaced by NaN; ii) data rows were removed when position data was NaN; iii) data rows were removed when flow speed of the pumped system was below 5 L/min; iv) data rows were removed when salinity values were considered artifacts for the study area (salinity values lower than 26), associated to the transition between sensors; v) data rows were removed when internal temperature, salinity, chlorophyll-a, turbidity, and ship speed data was NaN; vi) one-minute averages were calculated to smooth the data. It is important to note that the data file includes measurements sampled at the stations (i.e., when ship speed is close to 0 kn). An overview of the chlorophyll-a concentrations and turbidity from both sensors is represented in Figure 3.

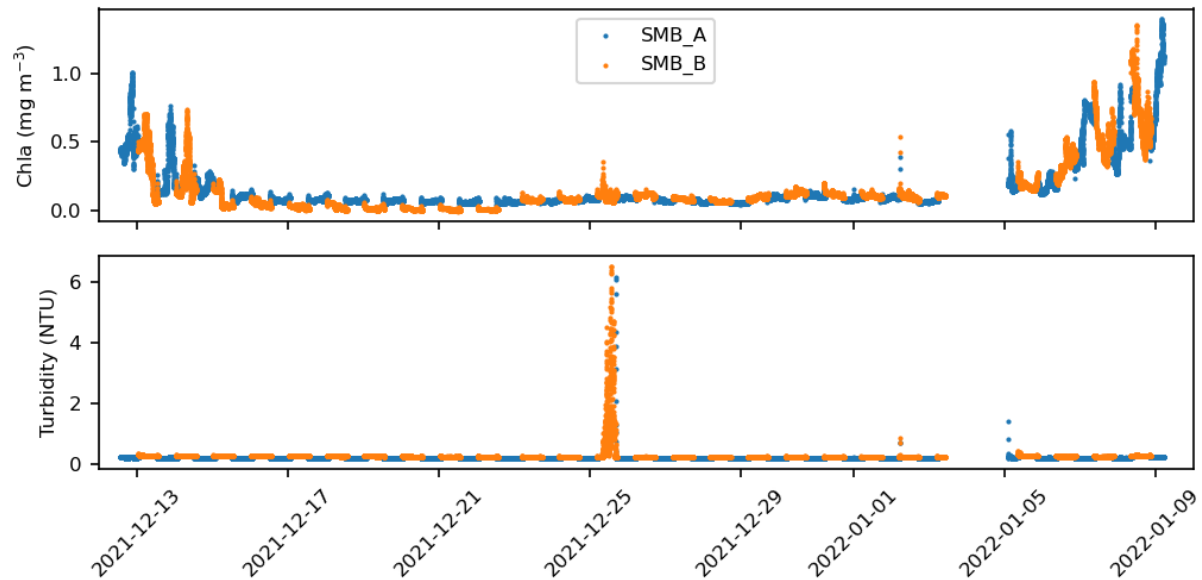


Figure 3 - Time series (one-minute resolution) of chlorophyll-a concentrations and turbidity acquired by the SMB_A (blue dots) and SMB_B (orange dots).

A comparison between underway and CTD chlorophyll-a and turbidity (for details about the CTD dataset, see the data processing report available in the OSIS portal) is shown in Figure 4. From this figure, it is possible to verify an offset between the underway turbidity sensors. In order to correct this data, and considering that the sensor SMB_B was malfunctioning at the beginning of the cruise, the turbidity data from sensor SMB_B was corrected based on data from sensor SMB_A by applying an offset resulting from the difference between both sensors (Figure 5). After this, we corrected the full time series of underway turbidity data by applying an offset resulting from the difference between underway and CTD turbidity values (from 8 m depth; Figure 6).

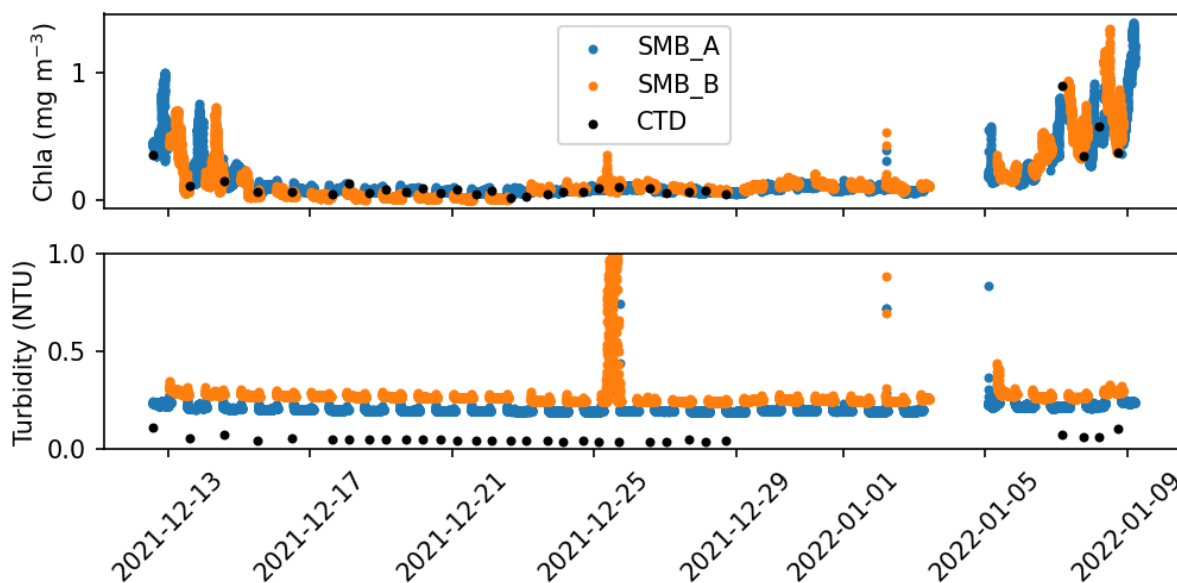


Figure 4 - Comparison between underway (blue and orange dots for SMB_A and SMB_B sensors, respectively) and CTD chlorophyll-a and turbidity data (from 8 m depth; black dots). Note that the turbidity scale was set to 1 NTU for better visualization of the offset between the underway and CTD values.

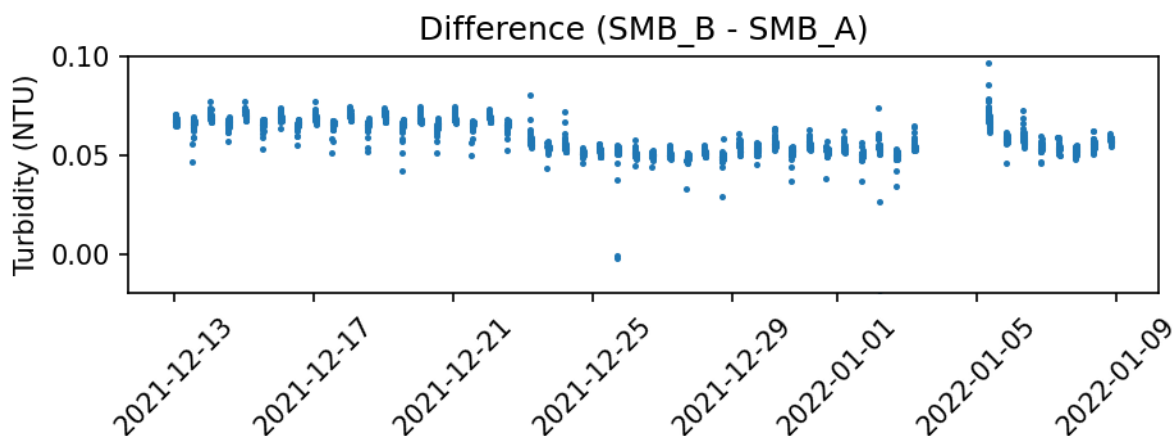


Figure 5 - Difference between turbidity values measured by the SMB_A and SMB_B sensors for common periods of time.

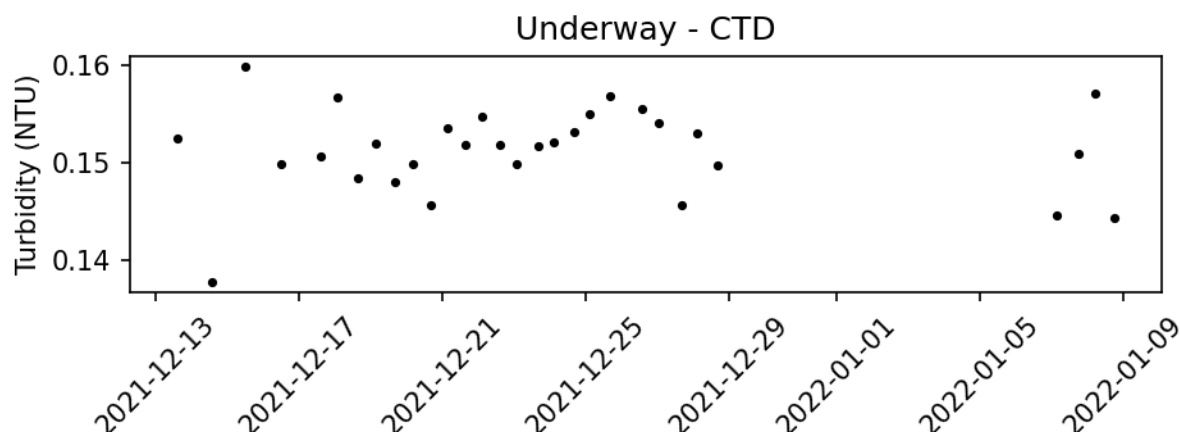


Figure 6 - Difference between turbidity values measured by the underway system and the CTD (from 8m depth).

Underway water samples were also taken to determine chlorophyll-a concentration by High-Performance Liquid Chromatography (HPLC; e.g. Zapata et al., 2000) analysis to be used in the calibration of chlorophyll-a fluorescence data. A comparison between underway chlorophyll-a with CTD chlorophyll-a, HPLC chlorophyll-a (from both underway and CTD samples), and satellite data (daily means at 4 km spatial resolution; OCEANCOLOUR_GLO_CHL_L3_NRT_OBSERVATIONS_009_032 from the Copernicus Marine Service⁴) was performed (Figure 7). From Figure 7, it is possible to verify that the underway data agreed quite well for the times when the ship was in the tropical Atlantic Ocean (between 22/12/2021 and 03/01/2022). Deviations can be seen for the beginning (between 12/12/2021 and 22/12/2021), in particular on data from the broken SMB_B sensor, and for the ending of the campaign (Pacific waters) when compared with the remaining datasets (HPLC samples and satellite data). In order to calibrate the underway chlorophyll-a data, the underway chlorophyll-a data from both sensors was compared with the HPLC data from the underway samples. Linear regressions for different periods were performed and the corresponding slope and offsets were applied to the underway chlorophyll-a data.

⁴ <https://marine.copernicus.eu/>

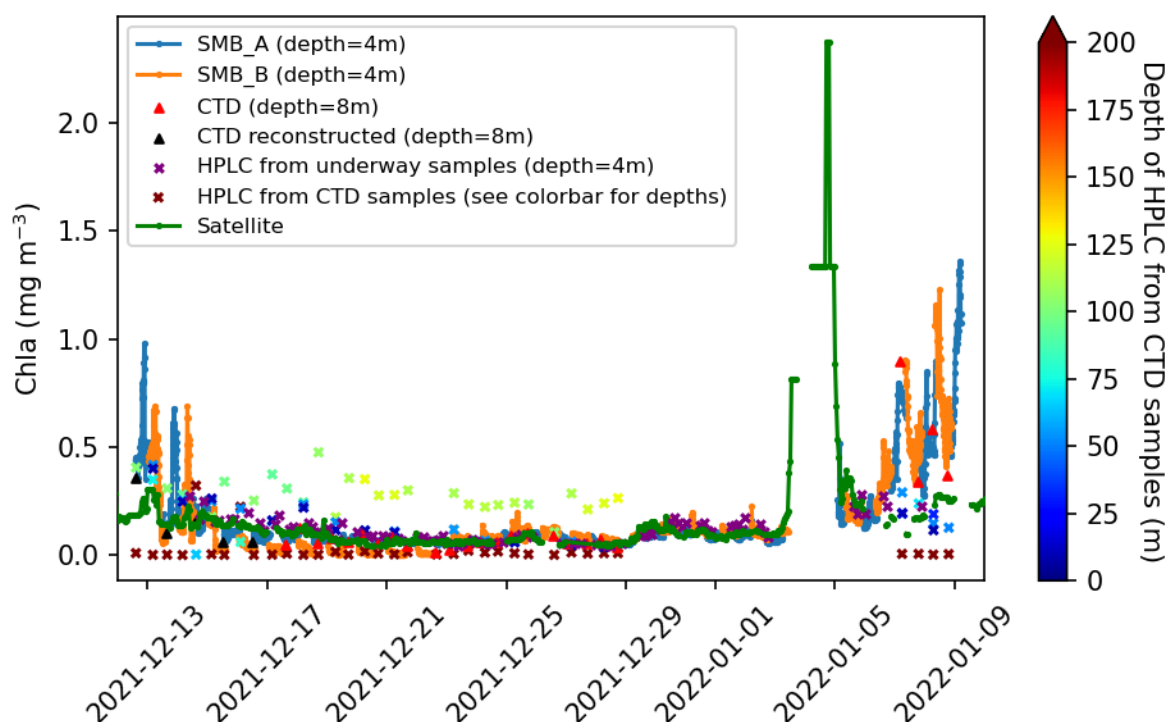


Figure 7 - Comparison between underway chlorophyll-a from both sensors (blue and orange dots for SMB_A and SMB_B, respectively), CTD chlorophyll-a (from 8 m depth; colored triangles), HPLC chlorophyll-a (from both underway and CTD samples; colored crosses), and satellite data (green dots).

From the comparison between underway chlorophyll-a (calibrated dataset) and CTD chlorophyll-a, HPLC chlorophyll-a, and satellite data (Figure 8), it is possible to verify that the underway dataset are much closer to the remaining datasets, except for the beginning (12/12/2021 to 15/12/2021) and ending (06/01/2022 to 09/01/2022) of the cruise. We believe that the higher concentrations at the beginning are probably associated with the possibility of algal growth in the stagnant water in the underway system while the ship was in the harbour, which takes some time to be removed from the system. This was already detected in some fluorescence time series from underway systems (please see the “Quality Control of Biogeochemical Measurements” document from Copernicus⁵). In relation to the higher concentrations at the ending of the cruise, in the Pacific waters, these are likely associated with a) changes in the phytoplankton physiology rather than higher phytoplankton abundance or b) optical interference associated with increased

⁵ <https://archimer.ifremer.fr/doc/00251/36232/88265.pdf>

water turbidity, as detected in the CTD chlorophyll-a data for the Pacific stations. For these reasons, these chlorophyll-a data periods got the flag 3 (i.e. bad data that are potentially correctable) following the “Quality Control of Biogeochemical Measurements” document from Copernicus (see Table I for the quality flagging scale). The remaining dataset was also checked and flagged after passing three quality control tests: i) Speed Test (valid speed value is considered in the range of the underway data minimum speed (5 kn) and maximum ship speed); ii) Frozen Value Test (over a range of 5 for all chlorophyll-a and turbidity values); and iii) Spike Test (UEDA, 2009). After these tests, some spike values still persisted, which seems to be related to the transition between sensors. In this sense, the data got the flag 4 in the first 8 minutes every sensor transition. A comparison between the final dataset flagged as 1 (valid data), 3 (bad data that are potentially correctable) and 4 (bad data) is shown in Figure 9.

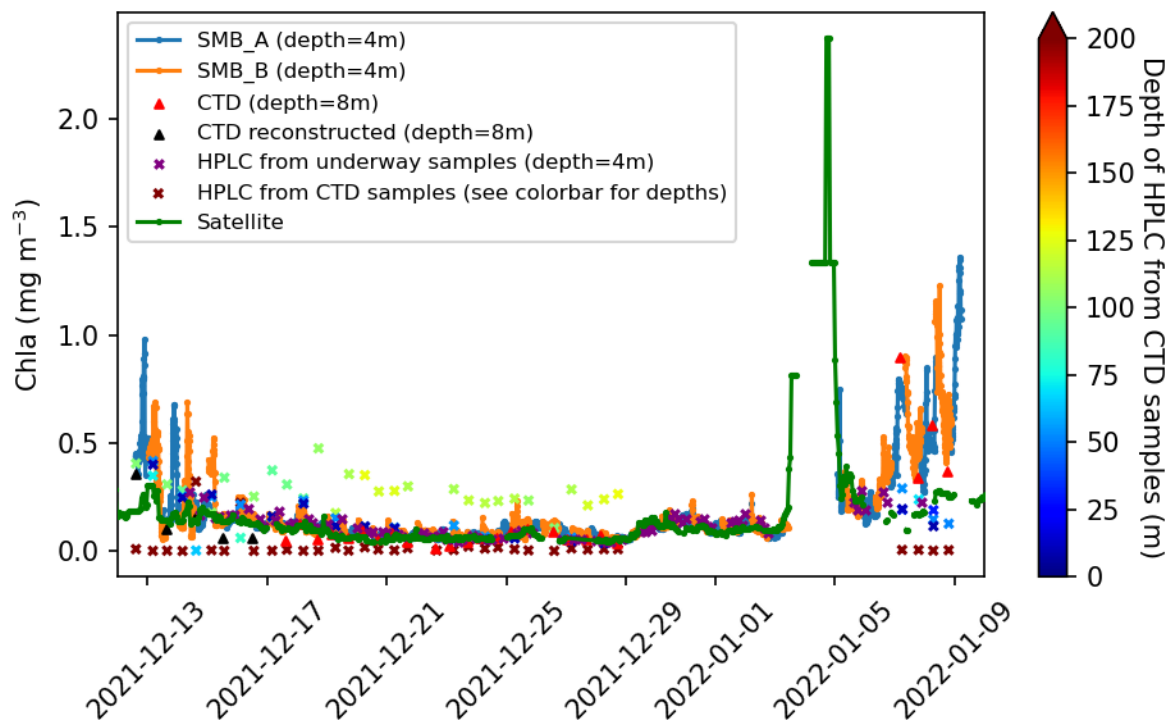


Figure 8 - Comparison between calibrated underway chlorophyll-a from both sensors (blue and orange dots for SMB_A and SMB_B, respectively), CTD chlorophyll-a (from 8 m depth; colored triangles), HPLC chlorophyll-a (from both underway and CTD samples; colored crosses), and satellite data (green dots).

Table I - Quality Flagging scale.

Code	Meaning	Comment
0	No QC was performed	-
1	Good data	All real-time QC tests passed.
2	Probably good data	-
3	Bad data that are potentially correctable	These data are not to be used without scientific correction.
4	Bad data	Data have failed one or more of the tests.
5	Value changed	Data may be recovered after transmission error.
6	Value below detection/quantification	The level of the measured phenomenon was too small to be quantified/detected by the technique employed to measure it. The accompanying value is the quantification/detection limit for the technique or zero if that value is unknown.
7	Nominal value	Data were not observed but reported (e.g. an instrument target depth)
8	Interpolated value	Missing data may be interpolated from neighbouring data in space or time.
9	Missing value	The value is missing.

The final data file is named as **SO287_underway_chla_turb**, in which columns are composed by time, coordinates (latitude and longitude), water depth, chlorophyll-a, turbidity, ship speed, and the active measurement container (SMB_A or SMB_B, or both).

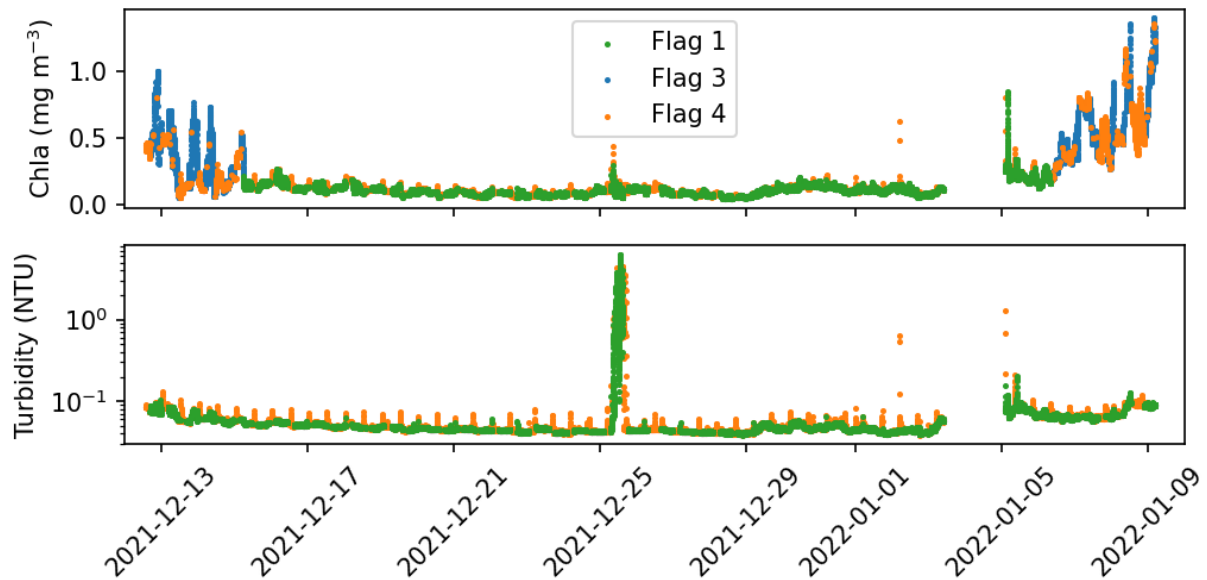


Figure 9 - Comparison between underway chlorophyll-a concentrations and turbidity data from the final data file flagged as 1 (valid data; green dots), 3 (bad data that are potentially correctable; blue dots) and 4 (bad data; orange dots). Note the logarithmic turbidity scale to emphasize the lowest values.

References

UEDA, T. 2009. A simple method for the detection of outliers. *Electronic Journal of Applied Statistical Analysis*, 67-76.

Zapata, M., Rodríguez, F., & Garrido, J. L. 2000. Separation of chlorophylls and carotenoids from marine phytoplankton: a new HPLC method using a reversed phase C8 column and pyridine-containing mobile phases. *Marine Ecology Progress Series*, 195, 29-45. <https://doi.org/10.3354/meps195029>