ALKOR-Berichte

Biogeo-optical and -chemical characterization of cyanobacterial blooms in the Baltic Sea for ocean colour satellite remote sensing

Cruise No. AL597

5 – 25 July 2023,
Kiel (Germany) – Tallinn (Estonia) – Kiel (Germany)
CYANO-OC

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1 Cruise Summary

1.1 Summary in English

Ocean Colour satellite remote sensing enables continuous and global monitoring of phytoplankton biomass and other water constituents in the upper layer of the ocean as well as of coastal and inland waters. The Baltic Sea is a particularly difficult water body to interpret from a remote sensing perspective; compared to other sea areas, it is very dark due to the high concentration of coloured dissolved organic matter brought in by many rivers and due to the limited water exchange with the North Sea. It also has intense cyanobacterial blooms in the summer months, which is not usual for temperate seas. This leads to large uncertainties in satellite products and limited usability of observational data. The measurement of specific optical properties in the field, especially of cyanobacteria, and the determination of biogeochemical properties are essential for the evaluation and further development of satellite products, e.g., regarding phytoplankton diversity or the marine carbon cycle.

During the ALKOR cruise, relevant bio-geo-optical and -chemical parameters were determined in the upper water layer and at the sea surface. High concentrations of cyanobacteria were detected and sampled. The cruising area could be flexibly optimised for match-ups with satellite data (with Copernicus satellites, but also with the German EnMAP mission), which resulted in an exceptionally large number of inter-comparison measurements for validation. The medium-term goal of this research is the development of novel Earth observation products to quantify biodiversity, detect environmental risks and better characterise the carbon cycle in the ocean.

1.2 Zusammenfassung

Die Satelliten-Fernerkundung der Ocean Colour ermöglicht ein kontinuierliches und globales Monitoring der marinen Biomasse und anderer Wasserinhaltsstoffe in der oberen Schicht des Ozeans, aber auch von Küsten- und Binnengewässern. Die Ostsee ist aus Fernerkundungssicht ein besonders schwierig zu deutendes Gewässer; im Vergleich mit anderen Seegebieten ist sie aufgrund vieler Flusseinträge und des limitierten Wasseraustauschs mit der Nordsee sehr dunkel (hoher Anteil von Gelbstoffen) und hat darüber hinaus intensive Algenblüten (die für die Ostsee typischen Cyanobakterien) in den Sommermonaten. Das führt zu großen Unsicherheiten in den Satelliten-Produkten und eingeschränkter Verwendbarkeit von Beobachtungs-daten. Die Messung grundlegender optischer Eigenschaften vor Ort, insbesondere von Cyanobakterien, und Bestimmung von biogeochemischen Eigenschaften sind essenziell für die Bewertung und Weiterentwicklung von Satellitenprodukten, z.B. im Hinblick auf Phytoplankton-Diversität oder den marinen Kohlenstoffkreislauf.

Auf der ALKOR Fahrt wurden relevante bio-geo-optische und -chemische Parameter in der oberen Wasserschicht und auf der Wasseroberfläche gemessen. Hohe Konzentrationen von Cyanobakterien konnten aufgespürt und beprobt werden. Das Fahrtgebiet konnte flexibel für Match-Ups mit Satellitendaten (vor allem mit Copernicus Satelliten, aber auch der deutschen EnMAP Mission) optimiert werden, wodurch außergewöhnlich viele Vergleichsmessungen für Validierungszwecke zustande gekommen sind. Das mittelfristige Ziel dieser Forschung ist die Entwicklung neuartiger Erdbeobachtungs-produkte zur Biodiversität, der Erkennung von Umweltrisiken und der besseren Charakterisierung des Kohlenstoffkreislaufs im Meer.

2 Participants

2.1 Principal Investigators

Name	Institution
Hieronymi, Martin, Dr.	Hereon
Röttgers, Rüdiger, Dr.	Hereon
Alikas, Krista, Prof. Dr.	University of Tartu
Kratzer, Susanne, Prof. Dr.	Stockholm University

2.2 Scientific Participants

Name	Discipline	Institution
Hieronymi, Martin, Dr.	Marine Optics / Chief Scientist	Hereon
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Bi, Shun, Dr.	Marine Optics	Hereon
Burmester, Henning	Marine Optics	Hereon
Novak, Mike	Marine Optics / PhD candidate	Hereon
Thölen, Claudia	Marine Optics / PhD candidate	University of Oldenburg
Alikas, Krista, Prof. Dr.	Marine Optics	University of Tartu
Roux, Pauline, Dr.	Marine Optics	Nantes University
Ansko, Ilmar	Marine Optics	University of Tartu
Rahn, Ian-Andreas	Marine Optics / PhD candidate	University of Tartu
Kratzer, Susanne, Prof. Dr.	Marine Optics	Stockholm University
Pramlall, Sejal	Marine Optics / PhD candidate	Stockholm University
Bravo, Vicky	Marine Optics / Intern	Stockholm University

2.3 Participating Institutions

Hereon	Helmholtz-Zentrum Hereon (Germany), Institute of Carbon Cycles, Departments of Optical Oceanography & Coastal Productivity
University of Oldenburg	Carl von Ossietzky Universität Oldenburg (Germany), Institute for Chemistry and Biology of the Marine Environment, Group of Marine Sensor Systems
Stockholm University	Stockholm University (Sweden), Marine Remote Sensing Group
University of Tartu	University of Tartu (Estonia), Tartu Observatory, Department of Remote Sensing
Nantes University	Nantes Université (France), Institut des Substances et Organismes de la Mer, Group of Remote Sensing, Benthic Ecology and Ecotoxicology

2.4 Contributors not on Boards

Several people have been involved in the organisational and scientific realisation of the campaign, from Hereon these are: Daniel Behr, Kerstin Heymann, Dr. Yoana G. Voynova, Martina Gehrung, and Ingo Kühnel. Dr. Gerald Moore (Bio-Optika, UK) helped with preparation of the radiometers of the Swedish team. Dr. Kersti Kangro, from the University of Tartu, is acknowledged for phytoplankton community composition analyses.

2.5 Captains

Hero Nannen	from Kiel to Tallinn, 5 – 15 July 2023
Jan Peter Lass	from Tallinn to Kiel, 15 – 25 July 2023

3 Research Program

3.1 Description of the Work Area

The starting and ending point of the journey was Kiel (Germany), a change of personnel was planned for Tallinn (Estonia); see Fig. 3.1 for the cruise track. The regional focus of the expedition was on Swedish, Estonian, and Finnish waters. The operation area includes the Arkona Basin, Bornholm Basin, Western and Eastern Gotland Basin, Northern Baltic Proper and Gulf of Finland. The main working area was around the island of Gotland. The actual route of the ship was determined by the overflight prediction of satellites (with focus on Copernicus satellites and EnMAP), but also significantly by current weather forecasts (especially regarding wind and cloud cover) and by economic navigation. Cyanobacteria occur every year in the summer in the central Baltic Sea; also, this year, as can be seen well from the satellite Chlorophyll-a map for the period of the cruise (Fig. 3.2). Accordingly, the travel time was chosen perfectly (granted).

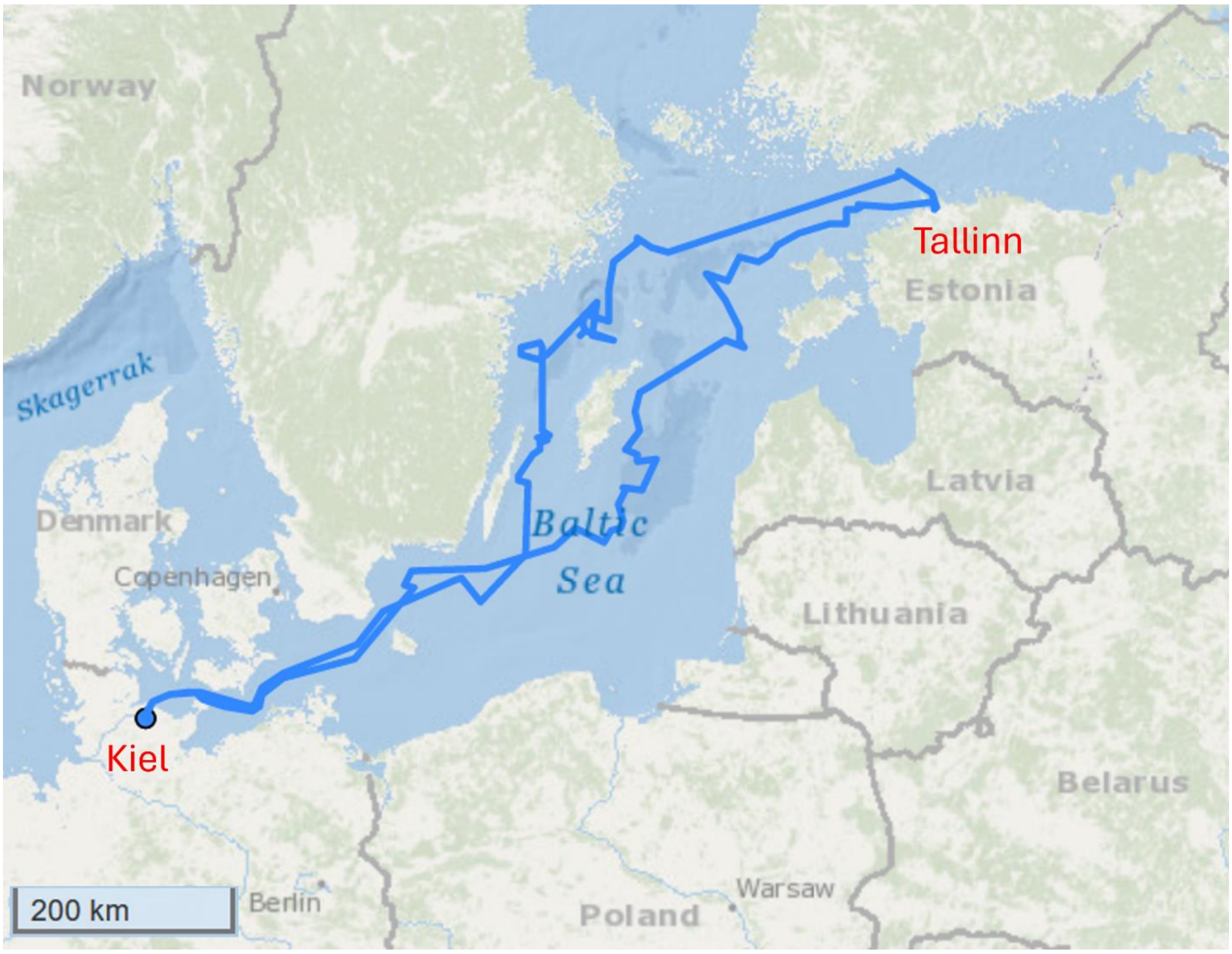

Fig. 3.1 Cruise track of AL597.

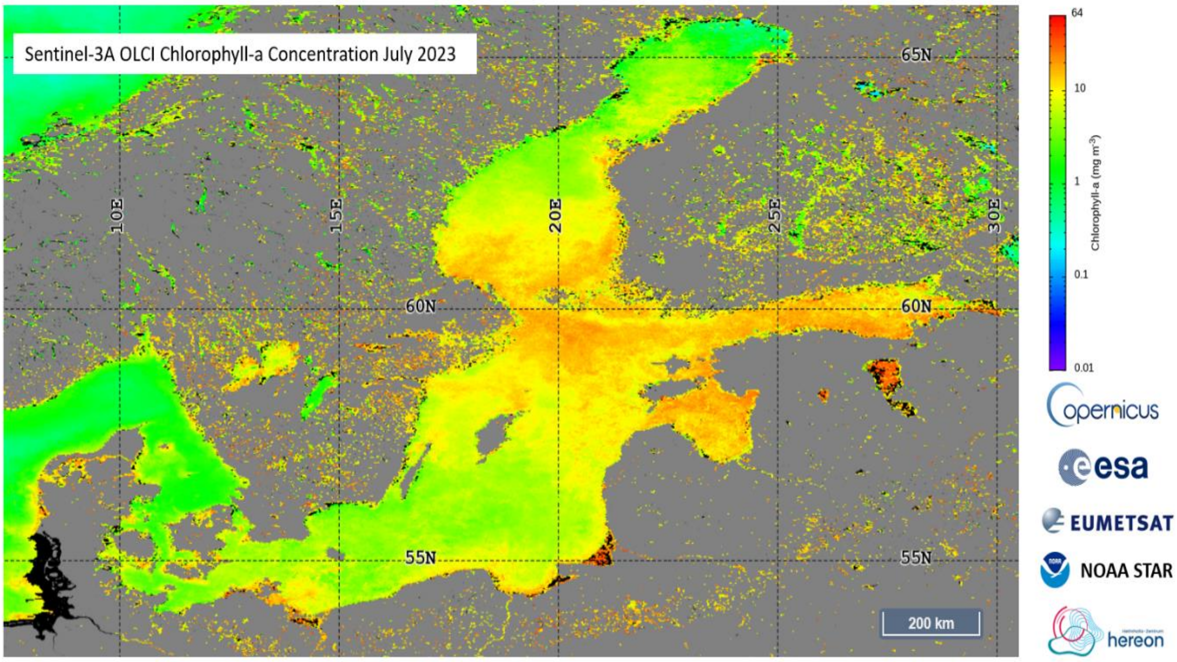

Fig. 3.2 Monthly averaged Chlorophyll-a concentration for July 2023 derived from Sentinel-3 OLCI satellite data.

3.2 Aims of the Cruise

The overall objective of the campaign is to improve and further develop satellite-based ocean colour products. The shipboard in situ measurements took place in a sea area that is particularly exposed to uncertainties for ocean colour, namely the Baltic Sea proper with relatively high concentrations of coloured dissolved organic matter (CDOM) and cyanobacteria. From a remote sensing perspective, the Baltic Sea is considered an extreme Case-2 water body (Hieronymi et al., 2016). The specific objectives of this cruise were 1) to perform high-precision hyperspectral measurements of chlorophyll- and mass-specific properties of cyanobacteria and other algae, 2) radiometric characterisation of water masses inside and outside accumulated cyanobacteria, 3) to investigate the stratification and vertical variability of optical properties, 4) to determine concentrations of carbon, pigment distributions and biogeochemical properties, 5) to test and compare of new optical instruments, and 6) to achieve a maximum of match-ups with various satellite missions.

3.3 Agenda of the Cruise

The journey took three weeks with a scheduled stop and change of personnel in Tallinn. Essentially three stops were scheduled per day at sea, approx. 8:30, 12:00 and 15:00 ship time. Due to the time-consuming analyses of water samples, Zodiac cruises with sampling of the sea surface microlayer were only realized at the first two stations, otherwise all measurements were carried out during the stations. If weather conditions allowed, transect cruises were carried out between the stations during the day.

In accordance with the agreements in the research proposal, we have strictly followed the Principles for Responsible Marine Research defined by KDM, DFG, and OSPAR to avoid unnecessary environmental and ecosystem disturbances. The impact of the conducted work to the environment can be considered as negligible small. We took water samples, but no sediment samples and we did not catch any fish. All instruments were recovered at the end of the cruise. There were no activities, which could lead to physical, chemical, biological, or geological changes or damage of marine habitats. Moreover, during the cruise, care was taken to minimize fuel consumption by traveling slowly and over short distances.

4 Narrative of the Cruise

Arrival and boarding went smoothly. However, we had a lot of devices and equipment, some of which had to be installed on the forecastle and in the mast. This makes setting up the measuring systems and securing the equipment and freight time-consuming. If the conditions are calm, it is normally possible to carry out the installations on ships that are already underway, which was the plan. However, a severe storm was approaching Kiel and the shipping area, which is why we postponed the departure by one day. This allowed us to complete the set-up and tests safely. We started our journey on Thursday in calm winds and good conditions.

The main aim of the expedition was to achieve as many match-ups as possible with satellite data, i.e. to combine in-situ measurements at sea with cloud-free Earth observation data from space. The daily program was therefore determined by three stations and transect passages between the waypoints, which were coordinated with overflight forecasts. This resulted in an unusual routing with curved sections of the journey, which were based on the position of the sun relative to the reflectance measurement systems at the bow of the ship. At the beginning of the trip, we were very lucky with the weather, so that many match-ups were successful.

The further north we moved, the more frequently large scum appeared on the sea surface, which reduced the surface roughness and therefore became visible as bright stripes. In the prevailing weak wind conditions, floating cyanobacteria often accumulated here. Water samples of the sea surface microlayer and underlying water layer were taken from the inflatable boat and analysed in the laboratory, primarily bio-geo-optically.

On the first leg of the journey, we had almost ideal measurement conditions for our research program. Above all, these included calm seas and a cloudless sky for undisturbed match-ups with satellite images. The stations were chosen to match several satellite overflights, which usually take their images around midday. The focus was on images from the *Ocean and Land Color Instruments* (OLCI) on the Sentinel-3A & B satellites. OLCI has an image width of 1270 km with 300 m pixel resolution and has 21 spectral bands. Images from the German hyperspectral satellite mission EnMAP were requested specifically for this trip to validate derived satellite products. Here the image width is 30 km with a resolution of 30 m, the instrument covers the spectral range from 420 to 1000 nanometres in 95 channels. On July 12, we were in areas with highly heterogeneous algae concentrations, which was also recorded by Sentinel-2 MSI; the *MultiSpectral Imager* has a pixel resolution of up to 10 m. Further match-ups with the US-American MODIS, VIIRS and Landsat sensors were achieved. In this respect, some excellent reference measurements with satellite data had already been made during the first leg of the journey.

On the evening of July 14, we arrived in Tallinn, the Estonian capital. Two scientists and Captain Hero Nannen disembarked in Tallinn; four scientists and Captain Jan-Peter Lass came on board for the second leg of the voyage. The Maritime Days took place in Tallinn that weekend, a family festival with many events, water sports, regattas, stage shows and many ships in the harbour. On Saturday, RV ALKOR was decorated with flags and opened to visitors between 10:30 and 14:30. Some scientists, especially our Estonian colleague, explained the research equipment and answered questions about current research at sea. Many families took the opportunity to see the German research vessel. Overall, this event was very well received.

We left Tallinn on Sunday morning in a northerly direction and continued our research in Finnish waters. New on board was the group from Sweden from Stockholm University. They began setting up their measuring equipment on Saturday, and on Sunday the equipment was tested at the three stations in order to try out procedures and optimize station operations. In calm weather conditions, some of the devices can be deployed in the water at the same time, allowing parallel measurements to be carried out and station times to be reduced. However, in heavy seas, as on the following Monday, not all measurements could be carried out, including the sea surface micro-layer sampling from the inflatable boat. Unfavourable wind conditions were forecasted for the coming days, so the route planning was changed somewhat.

The weather conditions changed generally in the last week; there was often significantly more wind and thus mixing of the upper water layer, as well as breakup of enriched biogenic surface films and cyanobacteria patches. There were also more heterogeneous cloud conditions, which made the reflectance measurements more difficult at times. Occasionally the cruise track, which was selected according to possible satellite match-ups, had to be changed for better wind and cloud conditions, but this worked very well. Relatively high concentrations of algae on the surface were mixed a little deeper by the waves. Clearly visible larger accumulations of cyanobacteria colonies, which we were able to observe particularly in the second week, were presumably broken up and fragmented - in any case, they could no longer be observed after the large-scale wind mixing, although we were also in other sea areas at that time.

We moved in visually similar water masses over the past week, with consistent specific absorption and scattering properties, indicating similar phytoplankton communities and covariances of constituents. On Sunday it rained for some time, from which rainwater samples were taken on deck, in addition to sampling the sea surface microlayer, where rain input plays a role. At noon in calm conditions, we were able to take samples of the microlayers again in clearly recognizable surface films. Sunday was also the last day on which the regular station program was carried out.

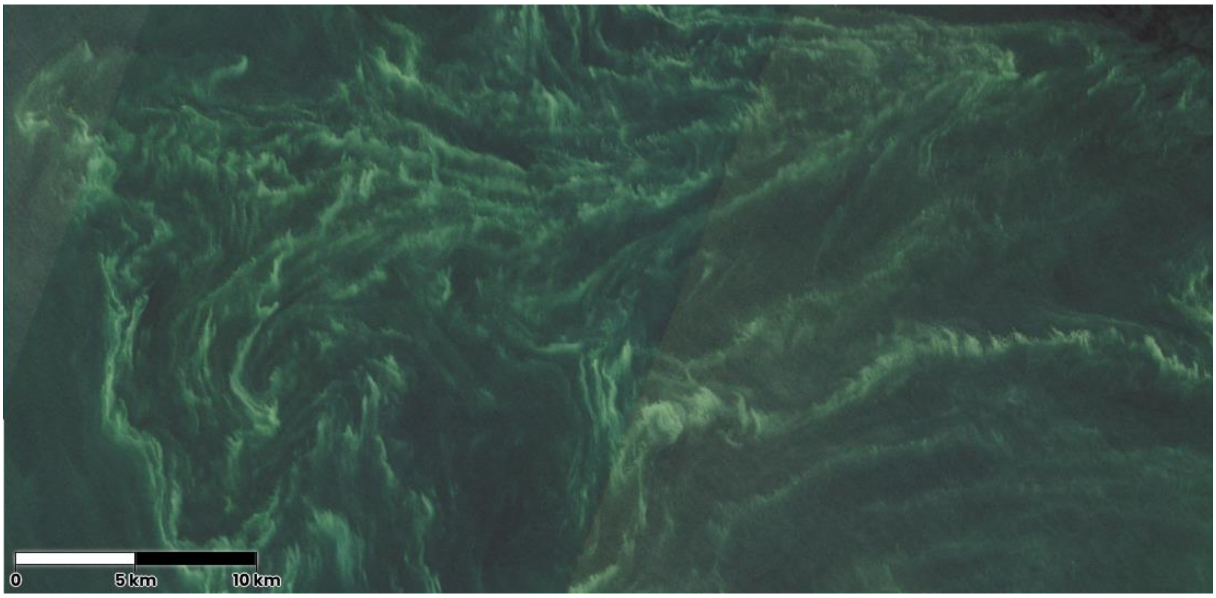

Fig. 4.1 Sentinel-2 MSI true colour image of the research area from July 12, 2023 (image extracted from the Tarkka service by the Finnish Environment Institute SYKE, https://tarkka.syke.fi/eo-tarkka/map/?ver=0&time=2023-07-12&style=opt&bbox=5.18547,53.62274,36.75371,61.67443&data=d-bm-esri,d-s2,d-lc&coll=call&lang=en).

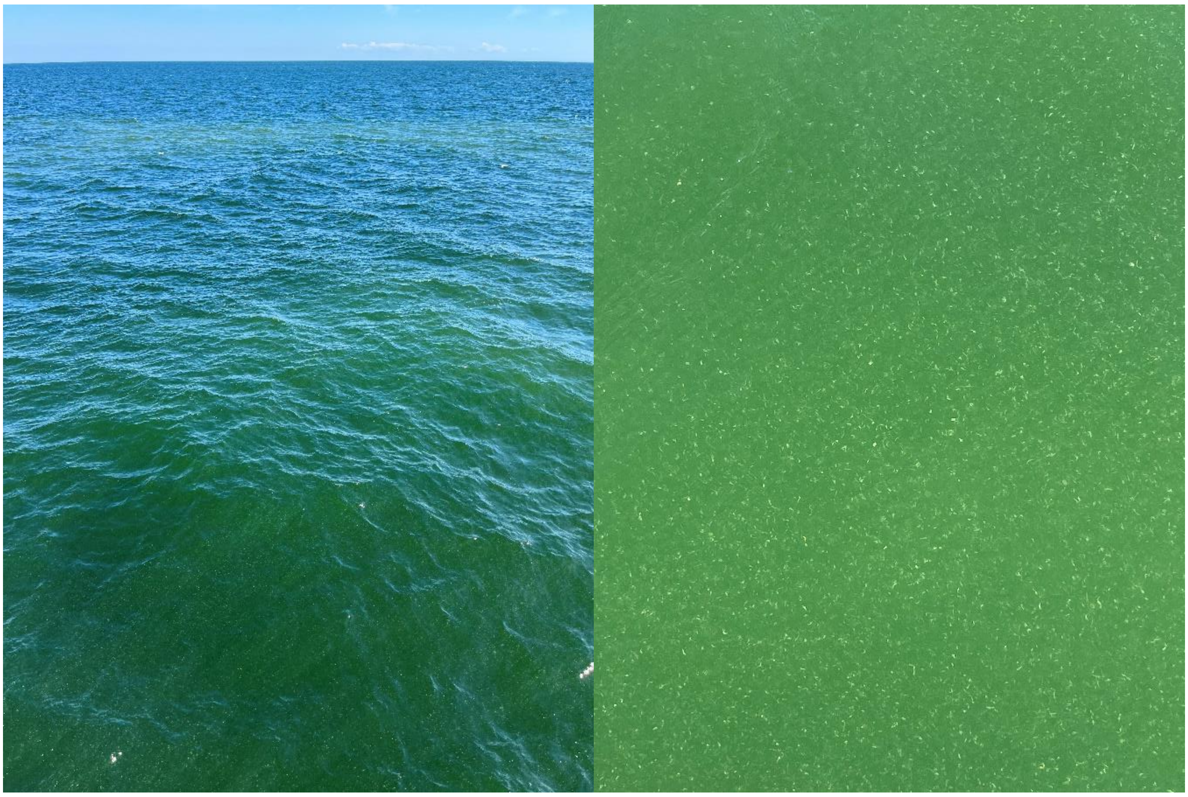

Fig. 4.2 Noticeably different water masses with sometimes very high algae concentrations and large-sized algae patches (Photos: M. Hieronymi).

Fig. 4.3 RV ALKOR open to visitors during Tallinn Maritime Days (Photos: M. Hieronymi).

5 Preliminary Results

5.1 Underway Measurements

5.1.1 Autonomous Measurements for Water Analysis

(Yoana G. Voynova, Martina Gehrung (both not on board), Martin Hieronymi)

Apart from the numerous parameters measured with the ship's own systems and made available directly in the DSHIP, other water parameters were measured in a flow-through mode throughout the voyage. A mobile version of the FerryBox, the Pocket FerryBox (4H-Jena Engineering, Germany), was deployed during AL597. This is smaller version of the normal FerryBox installations Hereon operates on ships of opportunity or fixed stations. The aim of this deployment was to observe the biogeochemical variability in surface waters, and to relate the measurements to satellite data, with a focus on different algal groups. Our goal during this cruise was to capture the variability of the surface Chlorophyll fluorescence data (TriOS NanoFlu, Germany), and data from the Algal Online Analyzer, AOA (bbe mohldaehnke, Germany), with the changes driven by small-scale physical variability (salinity, temperature), and of the biological primary production (dissolved oxygen, pH, CDOM). In addition, we took discrete water samples for nutrient analyses, specifically concerning the different algal groups. The Pocket FerryBox is relatively small, and does not provide automatic cleaning, but it can accommodate additional instruments, as seen here where the AOA instrument, is mounted to the left-hand side (Fig. 5.1).

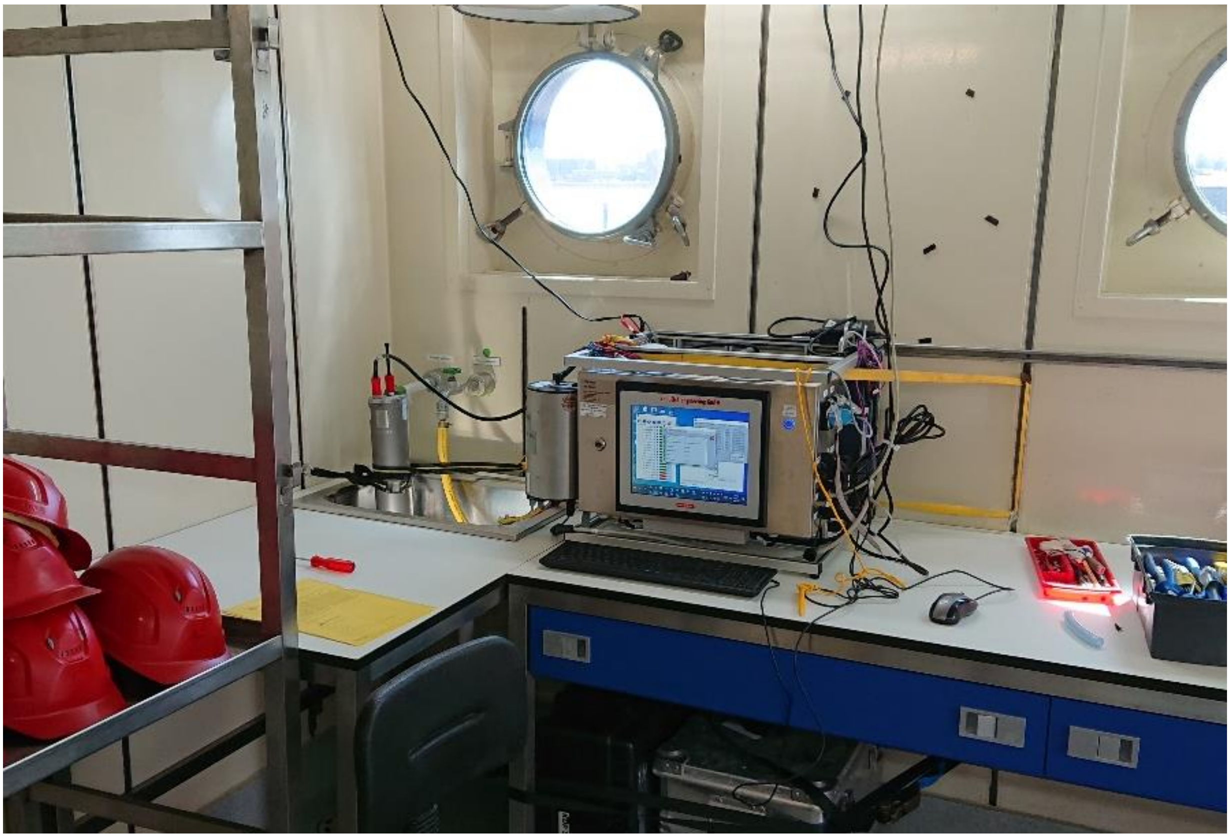

Fig. 5.1 Pocket FerryBox with Algal Online Analyser (AOA) sensor on the side of the FerryBox (Photo: M. Gehrung).

We were able to capture some of these dynamics in the preliminary FerryBox surface data, with gradients in dissolved oxygen, Chlorophyll fluorescence, temperature, pH, CDOM and salinity. However, additional analyses are necessary to further investigate this variability, and then compare them to satellite measurements and radiometer data. We are unable do see changes in Chlorophyll fluorescence, perhaps because the Chlorophyll maximum is deeper in the water column.

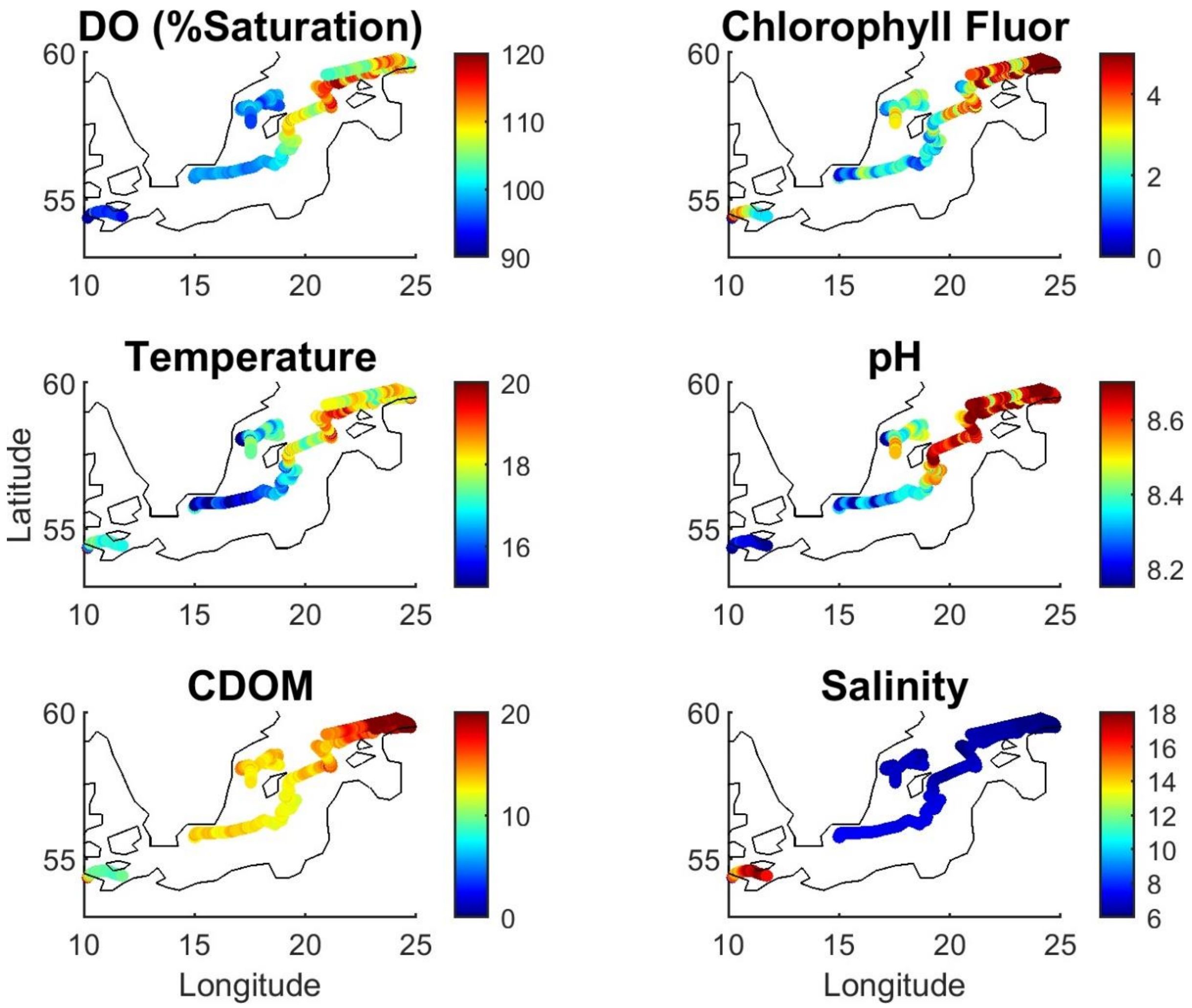

Fig. 5.2 Preliminary data of the Pocket FerryBox surface water parameters: dissolved oxygen (% saturation), Chlorophyll fluorescence, temperature (ºC), pH, CDOM fluorescence, and salinity (PSU). Variability in all parameters indicate the influence of both biological and temperature-driven features.

5.1.2 Radiometric Measurements Above Water

(Martin Hieronymi, Henning Burmester, Krista Alikas, Ilmar Ansko, Ian-Andreas Rahn)

The primary quantity determined by Ocean Colour satellite remote sensing is remote-sensing reflectance, R_{rs}. The associated above-water radiometric measurements were performed from the bow of RV ALKOR during the stations, but also in between during transit. When determining R_{rs}, directional radiance of the sky and the (undisturbed) water surface is measured, as well as the total downwelling irradiance, E_d. The same sensors (RAMSES, TriOS, Germany) from two groups were used, but also other sensors with different spectral resolution (Qmini, Broadcom, USA) or imaging spectroscopy (Cubert, Germany). The sensors were mounted on a common platform and aligned to the sun (e.g., at 90° or 135°) according to common protocols (Ruddick et al., 2019 a & b). Occasionally, R_{rs}-measurements were also conducted with a hand-held device (WISP-3, Water Insight, Netherlands). During transects, the direction of navigation was chosen in such a way that the sun was optimally oriented towards the measurement setup. Due to the changing sun position while the day, this resulted in curve-like tracks. During the measurements, environmental conditions like wind speed, cloud conditions, wave height, etc. were recorded and images from water surface and sky conditions were taken. In addition, a full-sky camera with a fisheye lens was used to draw conclusions about clouds and cloud cover. In direct sunlight, aerosol optical thickness was also frequently determined using hand-held *Microtops* Sun-photometer.

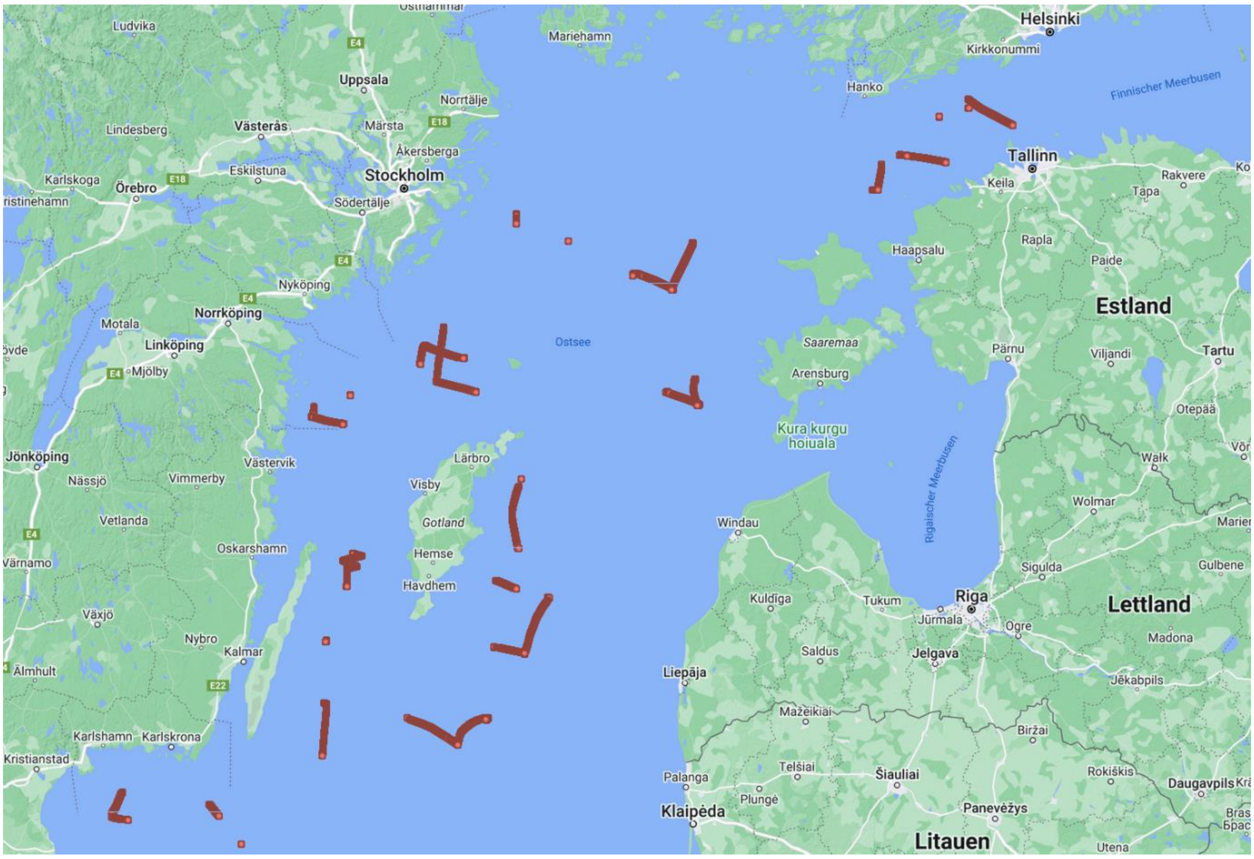

Fig. 5.3 Locations of remote-sensing reflectance measurements during stations and transects between stations for satellite comparison.

5.2 Works During Stations

5.2.1 Radiometric Measurements

(Martin Hieronymi, Henning Burmester, Krista Alikas, Ilmar Ansko, Ian-Andreas Rahn, Susanne Kratzer, Sejal Pramlall, Vicky Bravo)

In addition to the above-water reflectance measurements on the bow and in the mast, various radiometric quantities were measured in the water column and directly at the water surface to draw direct conclusions about the photosynthetically available radiation (*PAR*) in the water and to derive surface reflectance. These measurements were aimed at comparing various measurement protocols similar to Tilstone et al. (2020) and Zibordi et al. (2012), to investigate light polarization effects

(Hieronymi, 2016), and to test theories of the radiative transfer through the wavy water surface (Hieronymi, 2013; Bi et al., 2023). In each station, radiometric measurements were recorded for at least 15 minutes up to a few hours, depending on the conditions. Four different radiometric systems were used to measure the underwater light field. A *PAR* sensor (Sea-Bird Scientific, USA) was mounted on the CTD instrument frame to measure the light profile down to greater depths. The Hereon optical buoy was mostly deployed during the entire station duration; equipped with TriOS-RAMSES sensors, it measures upwelling radiance and downwelling irradiance just below the water surface. The TACCS is a setup of radiometers with seven channels for upwelling radiance, three channels for downwelling irradiance above the surface, and a chain of E_d -sensors (at 490 nm) placed at 2, 4, 6, and 8 m depth to derive the diffuse attenuation coefficient of downwelling irradiance, K_d(490). Both systems, the TACCS and Hereon optical buoy were deployed from the stern of the vessel and drifted away from the ship as to avoid ship-shading. Moreover, the team took profiles with the LI-COR (LI-COR Biosciences, Germany) measuring scalar *PAR* irradiance for deriving K_{dPAR}. An additional LI-COR planar irradiance deck sensor was deployed on top of the large frame on the aft of the research vessel; it is used to correct for the relative changes in downwelling irradiance when deriving K_{dPAR}.

Fig. 5.4 Left: TACCS radiometer deployed at sea (Photo: S. Kratzer). Right: Hereon optical buoy on deck (Photo: M. Hieronymi).

5.2.2 Profiling

(Rüdiger Röttgers, Henning Burmester, Shun Bi, Susanne Kratzer, Sejal Pramlall, Vicky Bravo, Martin Hieronymi)

At each station, the team determined the Secchi depth with different disks and visually matched the Forel-Ule number. The parameters are historical reference values about the turbidity and colour appearance of the water.

A 12-position water sampler frame was used for profiling the water column to just before the bottom, but to a maximum of 100 m depth. The frame is equipped with eight sampling bottles and a CTD that is additionally equipped with oxygen, chlorophyll fluorescence and turbidity sensors. Moreover, other bio-geo-optical sensors were mounted: several backscatter sensors (two Eco-VSF (Sea-Bird Scientific, USA) and a HydroScat-6 (HOBI Labs, USA)), two AC-S spectral absorption-attenuation meters (Sea-Bird Scientific, USA), a LISST-VSF scattering meter (Sequoia Scientific, USA), a LISST-Holo, and a PAR irradiance sensor. Bio-geo-chemical and -optical profiles were conducted at a low lowering speed of 0.1-0.3 m/s until the maximum depth. Water samples of 30-40 l were taken in the upper mixed layer in about 5 m water depth.

On the second leg of the cruise, another optical package was deployed, which allowed the top layer to be profiled more precisely. The instrument frame included an AC-9 (WetLabs, USA), a CTD sensor (SAI/VAS STD, Norway), a Volume Scattering Function meter (VSF-3, WetLabs, USA), a *PAR* sensor (Biospherical Instruments, USA) measuring scalar irradiance, a SeaPoint turbidity meter, a TriLux flurometer (Chelsea Technologies Group, UK) measuring Chlorophyll-a, phycocyanin and phycoerythrin.

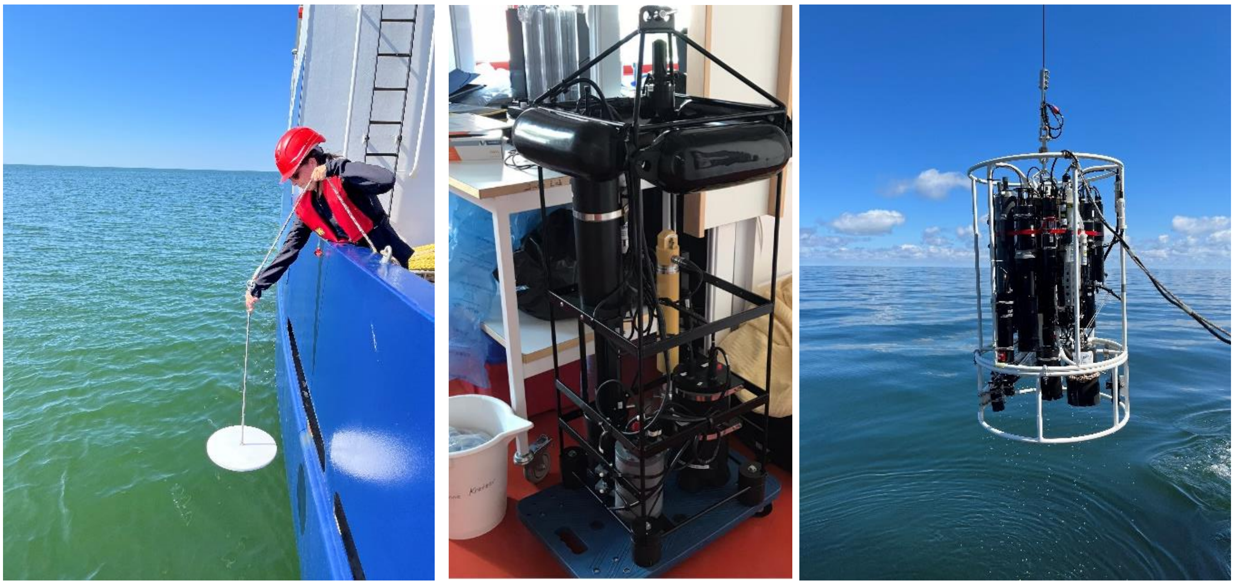

Fig. 5.5 Left: Deployment of the Secchi disk (Photo: M. Hieronymi). Centre: AC-9 optical package (Photo: S. Kratzer). Right: CTD water sampler and instrument frame (Photo: M. Hieronymi).

5.2.3 Sea Surface Microlayer

(Mike Novak, Claudia Thölen)

During most of the stations, the weather and sea state conditions were good for the use of the Zodiac. At some distance from the ship, special water samples of the sea surface microlayer (SML) samples were collected in an elaborate way by immersing a glass plate and skimming the liquid. The SML is a thin layer on the ocean's surface and has a maximum thickness of 1 µm. It is consistently enriched in biogenic surface-active organic material (surfactants) and acts as the skin of the sea where all fluxes, i.e. energy, gas, momentum between atmosphere and ocean pass though (Wurl et al., 2011). Two litres of SML were sampled on each Zodiac station. An additional two litres of underlying water (ULW or bulk) were sampled at each station. For the bulk water sampling a 2 L water bottle was manually submerged under the surface in about 50 cm depth, opened, filled, and closed under water to avoid contact with the SML. Some good samples with transparent slick (high SML accumulation) or accumulated algae could be collected. The laboratory investigations focused on the bio-optical properties of the organic substances in the SML and their fluorescence emissions; specially on the dissolved and particulate organic matter fraction (CDOM and POM) and in the living microalgae (phytoneuston).

Fig. 5.6 Left: The zodiac in action (Photo: M. Hieronymi). Centre: Slick at the surface smooths surface waves, stripes are visible (Photo: M. Hieronymi). Right: Nodularia spumigena surface accumulations (Photo: S. Kratzer).

5.3 On Board Laboratory Works

(Rüdiger Röttgers, Shun Bi, Mike Novak, Claudia Thölen, Pauline Roux, Krista Alikas)

The water samples were mainly analysed for their absorption and scattering properties. Essentially all spectral inherent optical properties (IOPs) were measured precisely with state-of-the-art methods with the aim of improving our theoretical understanding of bio-geo-optical modelling (Bi et al., 2023). Another objective was also to compare different measurement systems and analysis protocols, but also the variation of results with the same devices from different groups. Water turbidity, for example, was measured with three portable devices made by HACH (USA).

Water samples collected from the upper layer (0-10 m) using the CTD were subjected to various filtration processes on board to facilitate subsequent detailed and time-consuming analysis later on. These filtration steps were crucial for assessing phytoplankton biomass, taxonomic group composition, carbon, suspended particles, and other parameters. Additionally, samples from the CTD water at all stations were used for HPLC (High Performance Liquid Chromatography), CDOM (Chromophoric Dissolved Organic Matter), FDOM (Fluorescent Dissolved Organic Matter), surfactants, POC (Particulate Organic Carbon), and DOC (Dissolved Organic Carbon) analyses. Filtration was also performed to measure particulate absorption in the near-infrared spectral region (Röttgers et al, 2014) and other absorption components in the QFT-ICAM (Röttgers and Doerffer, 2007; Röttgers et al, 2016). For selected stations, filtration was carried out to determine the total suspended matter (TSM) concentration, filtering different volumes. In addition, samples from the sea surface microlayer (SML) and subsurface (bulk) were filtered for HPLC, POC and DOC analyses. A particle size fractionation was performed on part of the CTD water, and samples of different sizes were processed accordingly.

Optical measurements were carried out on surface water samples obtained from the CTD, zodiac-water, and size-fractionated water. Various prototype instruments were used to determine absorption and backscatter properties. Among them the PSICAM (Point-Source Integrating Cavity Absorption Meter), the QFT-ICAM systems and a setup featuring three LWCC (Liquid Waveguide Capillary Cell) systems of varying path lengths to measure absorption properties. Flow imaging microscopy with a FlowCam (Yokogawa Fluid Imaging Technologies, USA) was deployed to obtain high-resolution images to analyse the shape, size, and count of sub-visible particles and microorganisms. Besides the characterization of prominent particles like phytoplankton, detritus or sediments, the analysis can be used to obtain a particle size distribution.

All samples were immediately used to optical measurements after filtration, except for HPLC, NIR, POC, and DOC samples, which were preserved for further analysis in the home laboratory. HPLC and NIR samples were transferred to 2 mL Nalgene vials and Petri Slides, respectively, and were shock-frozen in liquid nitrogen, and later stored at -80°C for storage. POC and TSM filters were transferred to plastic Petri Slides and dried at 60°C. DOC samples were transferred to triple 50 mL glass ampoules or glass vials with Teflon-sealed cups and frozen at -20°C.

Table 5.1 Description of filtration items and **methods**

Item	**Description**
TSM	Total suspended particulate matter concentration – determined via gravitational technique using pre-combusted 45mm GF/F filters (Whatman) with a multiple (6x) steel filtration unit (Röttgers et al., 2014b)
POC	Particulate organic carbon concentration – using pre-combusted 25mm GF/F filters (Whatman) with a multiple (3x) steel filtration unit
DOC	Concentration of dissolved organic carbon – double filtration, filtrate through 45mm GF/F filters and then 0.22µm GSWP filter (Millipore)
HPLC	Concentration of phytoplankton pigments – high performance liquid chromatography, using pre-combusted 45mm GF/F filters (Whatman)
NIR	Particulate absorption coefficient in the near-infrared spectral region (NIR) – using pre-combusted 45mm GF/F filters (Whatman)
APM	Measurement of total particulate absorption – using pre-combusted 25mm GF/F filters (Whatman) for QFT-ICAM
CDOM	Chromophoric dissolved organic matter absorption – double filtration, filtrate through 45mm GF/F filters and then 0.22µm GSWP filter (Millipore)
FDOM	Dissolved organic matter fluorescence – filtration through 0.2 µm WWPTFE membrane

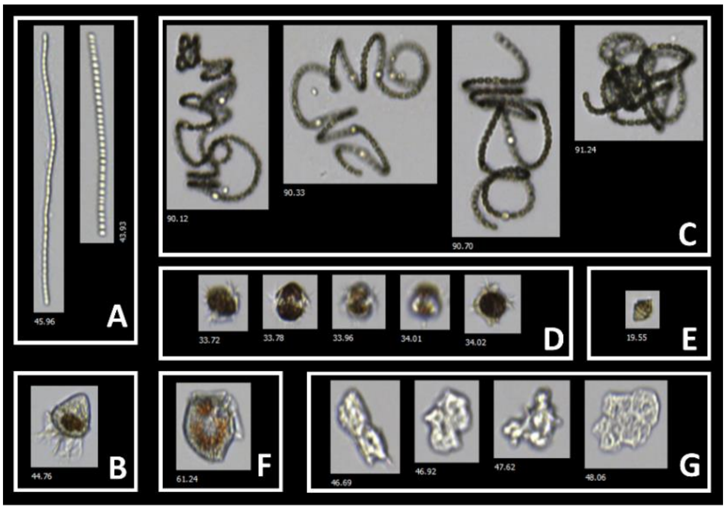

Fig. 5.7 Left: Flow imaging microscopy with a FlowCam. Right: Examples of FlowCam images of marine particles: A: Cyanobacteria, B: Ciliate, C: Cyanobacteria (Nodularia), D: Ciliate, E: Dinoflagellate, F: Dinophysis, G: unknown particles (Photos: C. Thölen).

5.4 Satellite Data

(Martin Hieronymi, Daniel Behr, Krista Alikas, Susanne Kratzer, Sejal Pramlall)

The main objective of the campaign was to generate complete optical validation data for a high number of satellite match-ups, which was achieved. Such measurements are used to validate atmospheric correction algorithms for ocean colour data (Hieronymi et al., 2023). The focus was on satellites of the European Copernicus programme with Sentinel-3 OLCI and Sentinel-2 MSI. The Ocean and Land Colour Instrument (OLCI) has an image width of about 1270 km with 300 m pixel size and 21 spectral bands. The Multi-Spectral Instrument (MSI) has about 270 km swath, up to 10 m resolution, but less relevant bands. Two satellites from each of the two satellite missions are currently in operational use, S3A & S3B and S2A & S2B.

In addition, images from the German hyperspectral EnMAP mission were ordered especially for this campaign. Attempting to create EnMAP match-ups has been the most restrictive aspect for the RV ALKOR navigation. EnMAP has a swath of 30 km, at 30 m pixel resolution, but hyperspectral data. Beyond the mentioned sensors, also other operational satellite sensors are of interest (e.g., the US America missions Aqua/MODIS, VIIRS/SNPP & NOAA, Landsat-8&-9/OLI, or the Japanese SGLI/GCOM). The in situ reflectance measurements in particular were carried out in such a way that they can be used for various band configurations of different satellite missions (Hieronymi, 2019).

The fundamental inter-comparison parameters are spectral remote-sensing reflectances from atmospherically corrected satellite images, i.e., the reference level is directly at the water surface. Typical water quality parameters are derived from this parameter: inherent optical properties, concentration of chlorophyll and (organic, inorganic, dissolved) carbon, light availability and attenuation in the water. Feedback on product quality will be communicated to EUMETSAT & ESA via the Sentinel-3 Validations Team. Furthermore, the data is used for the validation of other processing chains, e.g. ONNS (Hieronymi et al., 2017).

Table 5.2 Overview of achieved satellite match-ups (with limited use due to clouds etc. in grey).

Date	S3A-OLCI	S3B-OLCI	S2A-MSI	S2B-MSI	EnMAP	Landsat 8/9	MODIS	VIIRS
2023-07-06	09:28						x	x
2023-07-07	09:02	10:04		x			x	x
2023-07-08	08:36	09:38				x	x	x
2023-07-09	09:51	09:12	x		10:19		x	x
2023-07-10	09:25	08:46			10:44		x	x
2023-07-11	08:59			x			x	x
2023-07-12	08:32	09:34	x				x	x
2023-07-13	09:47	09:08			10:22		x	x
2023-07-14	09:21	08:42		x			x	x
2023-07-16	08:29	09:31	x			x	x	x
2023-07-17	09:43	09:05		x	10:26		x	x
2023-07-18	09:17	08:38					x	x
2023-07-19	08:51	09:53	x				x	x
2023-07-20	10:06	09:27					x	x
2023-07-21	09:40	09:01				x	x	x
2023-07-22	09:14		x			x	x	x
2023-07-23	08:47	09:49				x	x	x

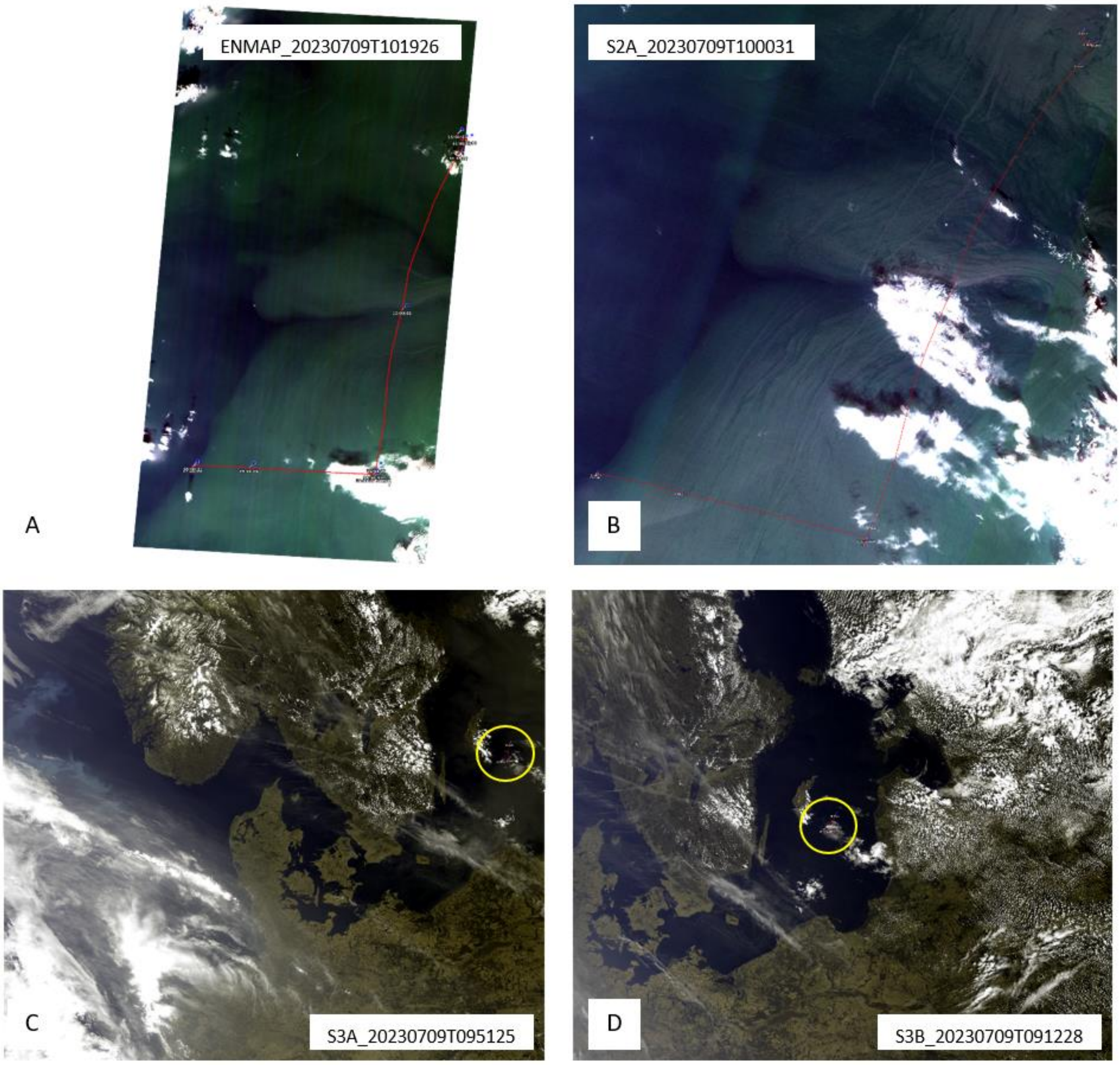

Fig. 5.8 Examples of satellite match-ups at the 9th of July southeast off the Island of Gotland. Red lines show the RV ALKOR transects with R_{rs} measurements. Level-1 (top-of-atmosphere) RGB images are shown for A) EnMAP, B) Sentinel-2A, C) Sentinel-3A, and D) Sentinel-3B (all with slightly different overpass times).

6 Station List AL597

On each day, the measurement programme was carried out at three stations, with start times of approximately 8:30, 12:00 and 15:00 ship time. CTD station profiles were carried out in the water column down to near the seabed, but to a maximum depth of 100 m. Radiometric parameters were often measured on transects between the three stations. In addition, there have been continuous measurements of water through-flow systems.

Station	Time (UTC)	Latitude (°N)	Longitude (°E)	Water depth [m]
AL597_0_Underway-1	2023-07-06 08:13:00	54.3543	10.168	13
AL597_1-1	2023-07-06 12:24:00	54.5308	11.2115	14
AL597_2-1	2023-07-07 07:02:00	55.71	15.1248	53
AL597_3-1	2023-07-07 10:17:00	55.7296	14.9506	47
AL597_4-1	2023-07-07 13:01:00	55.8752	15.0668	38
AL597_5-1	2023-07-08 06:56:00	56.319	18.1022	35
AL597_6-1	2023-07-08 10:37:00	56.1577	18.6362	100
AL597_7-1	2023-07-08 13:09:00	56.3187	18.9607	107
AL597_8-1	2023-07-09 07:03:00	56.7331	19.0218	147
AL597_9-1	2023-07-09 10:00:00	56.6968	19.3501	134
AL597_10-1	2023-07-09 13:08:00	57.0173	19.6135	168
AL597_11-1	2023-07-10 06:27:00	57.0706	19.2588	166
AL597_12-1	2023-07-10 10:23:00	57.3036	19.2909	124
AL597_13-1	2023-07-10 13:44:00	57.6984	19.3056	56
AL597_14-1	2023-07-11 06:29:00	58.1975	20.8642	45
AL597_15-1	2023-07-11 10:10:00	58.1223	21.2132	47
AL597_16-1	2023-07-11 13:05:00	58.2656	21.1683	46
AL597_17-1	2023-07-12 06:29:00	58.8377	20.4961	153
AL597_18-1	2023-07-12 10:03:00	58.7637	20.9301	86
AL597_19-1	2023-07-12 13:08:00	59.0178	21.1403	183
AL597_20-1	2023-07-13 06:29:00	59.3209	22.9164	113
AL597_21-1	2023-07-13 10:01:00	59.3087	23.1143	85
AL597_22-1	2023-07-13 14:10:00	59.4466	23.1481	94
AL597_23-1	2023-07-14 06:31:00	59.4974	23.3394	86
AL597_24-1	2023-07-14 09:59:00	59.4581	23.8274	88
AL597_25-1	2023-07-16 07:35:00	59.6575	24.539	73
AL597_26-1	2023-07-16 11:02:00	59.7471	24.0692	55
AL597_27-1	2023-07-16 13:41:00	59.7031	23.7589	61
AL597_28-1	2023-07-17 06:34:00	59.0279	19.8144	98
AL597_29-1	2023-07-17 10:03:00	59.1755	19.2568	49
AL597_30-1	2023-07-17 13:18:00	58.9476	18.7995	61
AL597_31-1	2023-07-18 06:25:00	58.3838	18.7033	173
AL597_32-1	2023-07-18 10:03:00	58.4533	18.2773	174
AL597_33-1	2023-07-18 13:14:00	58.3508	18.2362	147
AL597_34-1	2023-07-19 06:30:00	58.1955	18.829	107
AL597_35-1	2023-07-19 10:03:00	58.2492	18.4083	93
AL597_36-1	2023-07-19 13:04:00	58.5544	18.488	182
AL597_37-1	2023-07-20 06:31:00	58.0072	17.414	90
AL597_38-1	2023-07-20 10:05:00	58.0536	17.0763	64
AL597_39-1	2023-07-20 13:05:00	58.1756	17.4899	108
AL597_40-1	2023-07-21 06:33:00	57.2723	17.5227	83
AL597_41-1	2023-07-21 10:02:00	57.1895	17.4609	81
AL597_42-1	2023-07-21 13:04:00	57.0853	17.4543	87
AL597_43-1	2023-07-22 06:31:00	56.7634	17.229	88
AL597_44-1	2023-07-22 10:03:00	56.4052	17.216	50
AL597_45-1	2023-07-22 13:01:00	56.0984	17.1925	32
AL597_46-1	2023-07-23 06:34:00	55.5661	16.332	70
AL597_47-1	2023-07-23 10:06:00	55.7948	16.0064	61
AL597_48-1	2023-07-23 13:05:00	55.7448	15.7322	47

7 Data and Sample Storage and Availability

All water and filter samples obtained during the cruise were systematically labelled on board. All samples intended for longer-term storage were professionally archived immediately after the cruise. This includes frozen samples (-20°C and -80°C) where the majority of samples is stored at Hereon; additional samples are processed at Nantes University, University of Tartu and University of Oldenburg.

All digital data obtained during the cruise has been backed up by the respective groups. In addition, joint data are stored on different hard drives in different locations. Paper protocols filled out during the cruise were entered electronically continuously throughout the cruise, and thus fall under the electronic back-up scheme, but have also been conserved as hard copies to resolve possible data entry errors later on if needed.

All metadata of the cruise, including the ship's DSHIP data, were entered into the GEOMAR Ocean Science Information System (OSIS), which is managed by the Kiel Data Management Team (KDMT) and is intended for the permanent archiving of these data. The data are available under https://portal.geomar.de/metadata/cruise/show/363096 (related to AL597).

We encompass an open access data policy. The data from AL597 will be published in open access journals with the possibility to publish the data in a supplementary or additional data publication, together with the respective scientific article. Alternatively, the satellite-related match-up data will be made publicly available directly through the Copernicus Ocean Colour Database System (OCDB, https://ocdb.eumetsat.int), or through open access repositories (e.g., PANGEA) whilst ensuring the implementation of intellectual property rights of the PIs and the PhD students involved in the campaign.

Table 7.1 Overview of number of sub-datasets and responsible contact, who will make the data available.

Institute	Scientist	Number	Unit	Type of measurement
Hereon	Hieronymi, Martin	25	Transects	Above water radiometric measurements
Hereon	Hieronymi, Martin	48	Stations	Above water radiometric measurements
Hereon	Novak, Michael	33	Stations	Sea surface microlayer sampling
Hereon	Röttgers, Rüdiger	48	Stations	Measurement of turbidity and colour code
Hereon	Röttgers, Rüdiger	48	Stations	CTD-Stations with optical profiling <100 m
Hereon	Hieronymi, Martin	48	Stations	Radiometric measurements near the surface
Stockholm University	Kratzer, Susanne	20	Stations	Underwater radiometric profiles
Hereon	Voynova, Yoana		Minutes	Continuous FerryBox measurements
University of Tartu	Alikas, Krista	100	Stations	Sun-photometer measurements

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9 References

Bi, S., Röttgers, R., and Hieronymi, M., 2023. Transfer model to determine the above-water remote-sensing reflectance from the underwater remote-sensing ratio. Optics Express, 31(6), 10512-10524.

Bi, S., Hieronymi, M., and Röttgers, R., 2023. Bio-geo-optical modelling of natural waters. Frontiers in Marine Science, 10, 1196352.

Hieronymi, M. (2013). Monte Carlo code for the study of the dynamic light field at the wavy atmosphere-ocean interface. Journal of the European Optical Society-Rapid publications, 8.

Hieronymi, M., 2016. Polarized reflectance and transmittance distribution functions of the ocean surface. Optics Express, 24(14), A1045-A1068.

Hieronymi, M., Krasemann, H., Müller, D., Brockmann, C., Ruescas, A., Stelzer, K., et al., 2016. "Ocean Colour Remote Sensing of Extreme Case-2 Waters," in Proceedings of Living Planet Symposium (Prague: ESA SP-740).

Hieronymi, M., Müller, D., and Doerffer, R., 2017. The OLCI Neural Network Swarm (ONNS): a bio-geo-optical algorithm for open ocean and coastal waters. Frontiers in Marine Science, 4, 140.

Hieronymi, M., 2019. Spectral band adaptation of ocean color sensors for applicability of the multi-water biogeo-optical algorithm ONNS. Optics express, 27(12), A707-A724.

Hieronymi, M., Bi, S., Müller, D., Schütt, E. M., Behr, D., Brockmann, C., et al., 2023. Ocean color atmospheric correction methods in view of usability for different optical water types. Frontiers in Marine Science, 10, 1129876.

Röttgers, R., Häse, C., and Doerffer, R., 2007. Determination of the particulate absorption of microalgae using a point-source integrating-cavity absorption meter: verification with a photometric technique, improvements for pigment bleaching and correction for chlorophyll fluorescence. Limnol. Oceanogr. Methods 5: 1–12.

Röttgers, R., Dupouy, C., Taylor, B. B., Bracher, A., and Woźniak, S. B., 2014. Mass-specific light absorption coefficients of natural aquatic particles in the near-infrared spectral region. Limnology and oceanography, 59(5), 1449-1460.

Röttgers, R., Doxaran, D., and Dupouy, C., 2016. Quantitative filter technique measurements of spectral light absorption by aquatic particles using a portable integrating cavity absorption meter (QFT-ICAM). Opt. Express 24: A1.

Ruddick, K. G., Voss, K., Boss, E., Castagna, A., Frouin, R., Gilerson, A., et al., 2019a. A review of protocols for fiducial reference measurements of water-leaving radiance for validation of satellite remote-sensing data over water. Remote Sensing, 11(19), 2198.

Ruddick, K. G., Voss, K., Banks, A. C., Boss, E., Castagna, A., Frouin, R., et al., 2019b. A review of protocols for fiducial reference measurements of downwelling irradiance for the validation of satellite remote sensing data over water. Remote Sensing, 11(15), 1742.

Tilstone, G., Dall'Olmo, G., Hieronymi, M., Ruddick, K., Beck, M., Ligi, M., et al., 2020. Field intercomparison of radiometer measurements for ocean colour validation. Remote Sensing, 12(10), 1587.

Wurl, O., Wurl, E., Miller, L., Johnson, K., and Vagle, S., 2011. Formation and global distribution of sea-surface microlayers, Biogeosciences, 8, 121–135.

Zibordi, G., Ruddick, K., Ansko, I., Moore, G., Kratzer, S., Icely, J., and Reinart, A., 2012. In situ determination of the remote sensing reflectance: an inter-comparison. Ocean Science, 8(4), 567-586.