Colour and Light in the Ocean (CLEO) 2016

A Scientific Roadmap
from the
Workshop Organised by
ESA and PML
Held at ESRIN, Frascati, Italy
on 6-8 September, 2016

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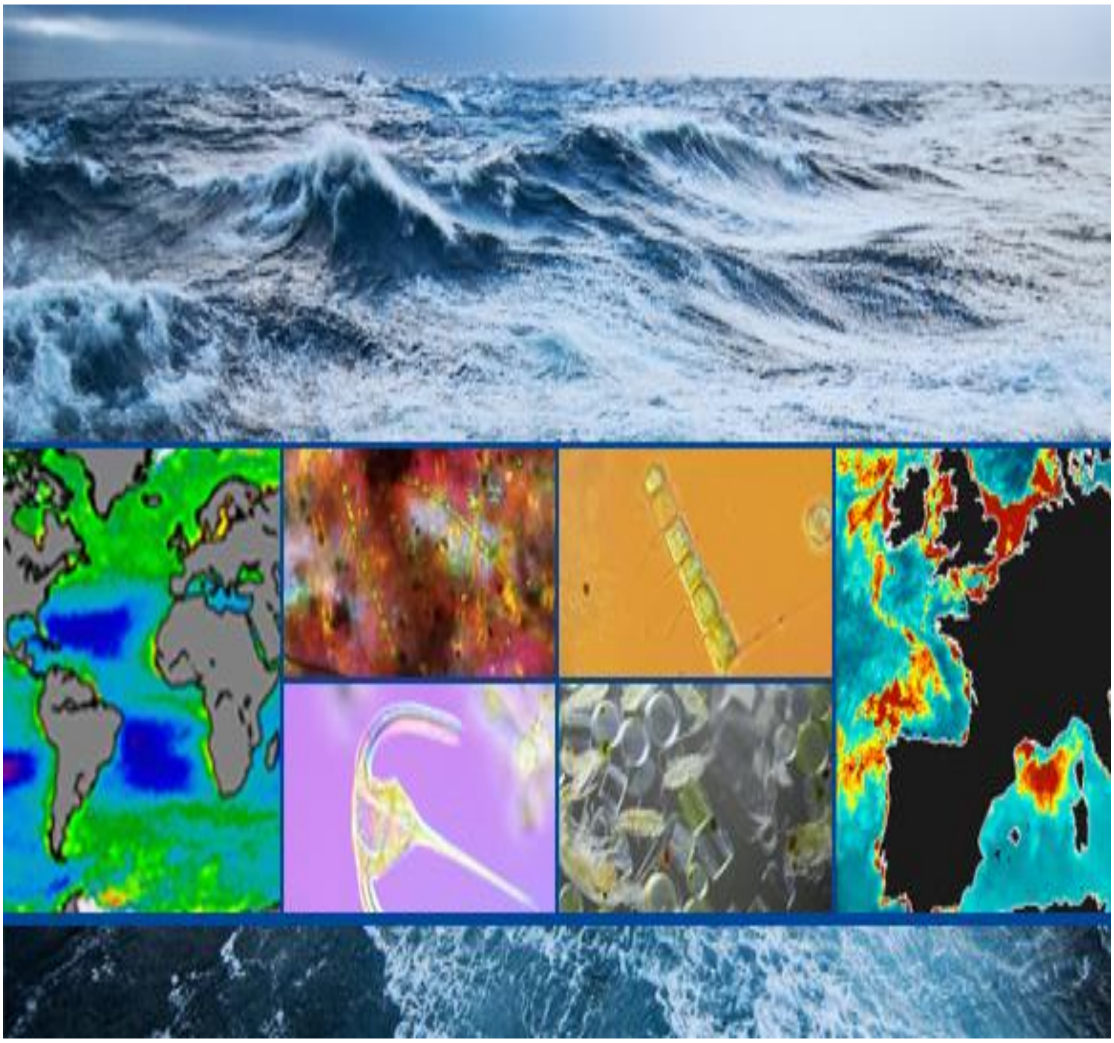

Executive Summary

The Colour and Light in the Ocean (CLEO) Workshop, organized by the European Space Agency (ESA) and the Plymouth Marine Laboratory (PML) was held on the ESRIN, the ESA Centre for Earth Observations, at Frascati, Italy on 6-8 September 2016.

The workshop is sponsored through selected SEOM (Scientific Exploitation of Operational Missions) projects, including:

- Pools of Carbon in the Ocean (POCO);
- Photosynthetically Active Radiation and Primary Production (PPP);
- Synergistic Exploitation of Hyper-and Multispectral Sentinel-Measurements to Determine Phytoplankton Functional Types (PFT) (SynSenPFT); and
- Extreme Case-2 Waters (C2X).

Additional partner projects of ESA are:

- Marine Photosynthesis Parameters from Space (MAPPS), a Pathfinder STSE (Support to Science Element) project; and
- Ocean Colour Climate Change Initiative (OC-CCI) through the CCI (Climate Change Initiative).

The objectives of the workshop were to:
Evaluate state-of-art:

- Exchange information with other relevant projects and activities
- Bring together remote sensing community, in situ data providers, modellers and other users
- Explore applications in marine ecosystem models

Plan for the future:

- Identify challenge areas and research priorities for future EO data exploitation activities
- Discuss key science issues and make recommendations to strengthen community engagement
- Shape ideas for potential new ocean- colour products to be developed in the era of the Sentinel-3 mission

The workshop was organized in five themes, developed around the activities of the sponsoring projects. Each theme had oral, poster and discussion sessions. The workshop attracted some 160 registered participants. The workshop served an important need to connect the community, to provide a forum for lively exchange of ideas, and to recommend priorities for future activities in a collective manner. The workshop brought together scientists working on development of novel products from ocean-colour data and the user community, including, notably, the modeling community.

One of the key outputs of the workshop is this report, which provides the Scientific Roadmap for future activities. Another planned outcome is a Special Issue on Colour and Light in the Oceans, to be published in the Journal *Frontiers in Marine Science*, which will highlight the major scientific results presented at the workshop.

Each section of the report, dealing with one of the themes of the workshop, is self-contained, but cross-references to other sections are provided where appropriate. Some recommendations found common resonance across sections, such as the need for continuous, consistent, ocean-colour data streams from satellites for long-term monitoring of the marine ecosystem; the need for an integrated approach, bringing together the remote-sensing community, the in situ data providers and the modeling community; the need to promote development of novel products and advanced sensors; and the importance of providing high-quality and uninterrupted support to the user community, through easy and free access to data and products. Each section discusses the current state of the art, identifies user requirements and gaps, and priorities for research in the short and medium terms.

The workshop served the important function of sounding the community's aspirations, and presenting them in a concise manner for ESA, through this Scientific Roadmap. One of the recommendations from the participants was that CLEO workshops be organized on a regular basis in the future, to develop the ocean-colour community, to promote exchange of new results and ideas, and to plan future activities.

We thank all workshop participants, keynote speakers, authors of the oral presentations and the posters, the Scientific Committee and the Organising Committee, and the Session Chairs for all their contributions to the workshop. For the logistical support and local organization and hospitality, we thank the ESRIN Graphics Bureau, Administration, Catering Service and the Events Office, especially Irene Renis, Anne Lisa Pichler and Giulia Vinicola.

Content

Session 1: Ocean Colour Applications for Climate Studies

Marcello Vichi, Shubha Sathyendranth, Meike Vogt, Cecile Rousseaux, Stephanie Dutkiewicz, Tiit Kutser, Victor Martinez, Carsten Brockmann, Didier Ramon, Oliver Clements, Trevor Platt, Mark Dowell, Peter Regner

1.1 Introduction

This report provides a scientific roadmap for the use of, and priorities for, ocean-colour products in climate research that emerged during the presentations (oral and poster) during the Climate Session and the corresponding Discussion Session at the CLEO workshop at ESRIN on 6-8 September, 2016. The climate-related sessions and discussions were organized within the context of the activities of the Ocean Colour Climate Change Initiative (OC-CCI) of ESA. The discussion session began with the following seed questions:

- Do existing merged ocean-colour time series data meet the requirements of the climate community? What can be done to serve better the needs of the user community in general and the modelling community in particular?
- What should be done to ensure the continuity of the data into the foreseeable future and to ensure that the quality of the time series reflects the latest developments in the field?
- What additional products should be added to the product streams to increase their usefulness *(cross–cutting issue)*?
- How can we communicate better to the broader community the importance of ocean colour in climate research?

Some of the participants from the modelling community (Stephanie Dutkiewicz, Cecile Rousseaux and Meike Vogt) gave written inputs to the report. The scientific roadmap presented here are provided largely from the perspective of the user community.

1.2 Requirements of the Extended Climate Community

Ocean colour data are essential to study the impact of climate change on marine and inland ecosystems (IPCC WG 1 and WG2). For vast areas of the ocean and millions of lakes that are not readily accessible by any other means, remote sensing provides the only avenue for monitoring status, variability and change. Another unique advantage of remote sensing is the large-scale perspective.

A fundamental application of ocean-colour data is for mapping the concentration of chlorophyll-a, the major photosynthetic pigment contained in phytoplankton: microscopic, free-floating plants in aquatic environments. The information on chlorophyll concentration can be used, along with data on light available for photosynthesis, to compute marine primary production, the process by which inorganic carbon in the ocean is converted to organic material. Phytoplankton are responsible for primary production of some 50 GT of carbon per year, globally, and are therefore an important player in the global carbon cycle. Ocean colour is also used to study export production: the fraction of primary production that is transported to the deep ocean. Ocean-colour data are also being used increasingly to map phytoplankton types and size classes from space (see section of report dealing with phytoplankton types): given the different roles of these phytoplankton types in ocean and inlan water bio-geochemical cycles, it is clear that such products are of interest to the climate community. More recent efforts in the ocean-colour community have explored the potential of ocean-colour data to quantify and map various components of dissolved and particulate pools of carbon in the ocean and inland waters (dealt with in the section devoted to Pools of Carbon in the Ocean, in the CLEO Report), with obvious interest for the climate community. Mapping the dissolved organic matter is especially important in lakes where more than 90% of carbon is usually in the dissolved form. Other applications include studies of cross-domain fluxes and interactions: ocean-atmosphere and land-ocean fluxes of carbon, ocean-cryosphere interactions and climate impact on the polar ecosystems. It must be noted that the carbon outgassed from lakes exceeds the carbon flux from land to oceans and the amount of carbon going to lake sediments is in the same order of magnitude than the flux of carbon from land system to oceans. Because of the fundamental importance of ocean colour and phytoplankton in the studies of the marine ecosystem and biogeochemical cycles, they are recognized as Essential Climate Variables (ECVs) by the Global Climate Observing System (GCOS).

Climate studies belong to three broad categories: detection, attribution and projection. The first two categories of studies have to rely on high-quality time series data to isolate any climate signal from natural variability. The third category requires accurate and synoptic information for setting initial conditions. Since the ocean environment is subject to variability at multiple scales, including decadal-scale variability, the time series has to be maintained in a consistent manner for multiple decades, to ensure confidence in attribution. Ocean-colour time series data produced by OC-CCI, which contains 18 years of uninterrupted, climate-quality data, is just getting long enough for isolating climate signals in some parts of the world oceans. At the same time, with its global reach, ocean-colour data serve to assess the current climate conditions, and to evaluate the impact of climate variability on the marine ecosystems, and the causes of variability, as a key to understanding potential future impacts, to underpin projections.

The functioning of the Earth System and the climate projections can be enhanced considerably when the data are used in conjunction with models. There are three types of climate models of relevance: Earth system models; coupled regional models and regional downscaling forced models. Ocean-colour data are essential for assessment of current climate conditions in Earth System models and parameterisations in process-based models. It is important to recognize that the dialogue between the observing community and the modelling community is a two-way interaction: models can inform Earth Observation Missions on required spatial and temporal resolution and length of time series required to capture climatic trends and variability. On the other hand, models should be able to reproduce key features in the satellite data.

Oceans play a considerable role in the global carbon cycle. Globally, oceans act a sink of carbon dioxide, taking up approximately 30% of the carbon dioxide emitted into the atmosphere. It is crucial that we understand the role of oceans and the effects that climate change may have on oceans and the carbon cycle. The role of inland waters in the global carbon cycle was completely ignored until the last IPCC report and there is still long way to go before the role of inland waters in the carbon cycle can be determined with higher accuracy. Various methods can be used to evaluate the pools of carbon in the oceans. From in situ sampling to satellite data and numerical models, each of these approaches provides a different piece of information in our understanding of the dynamics and variability of carbon pools and fluxes. While in situ data are often used to provide ground-truth datasets for calibration and validation of satellite data and parameterisation of numerical models, the collection of in situ data is labour intensive and can be expensive. Satellite data can provide global datasets but the variables that can be derived currently from ocean colour are limited to only some of the variables involved in the carbon cycle. Furthermore ocean colour data can be limited in time and space because of high solar zenith angle, interorbital gaps and the presence of aerosols and clouds that can be considerable in some regions. Finally, numerical models represent a best approximation of our understanding of processes driving the carbon cycle in the oceans; but they allow for global representation of only those variables whose processes are understood well enough to be represented in models. No models exist for inland waters. The assimilation of satellite ocean colour data in models can sometimes improve the models and provide an integrated framework that combines the benefits of both models and satellite data. Numerical models can also support the planning and design of field campaigns by conducting simulation experiments of various sampling strategies as well as by providing forecasts of the conditions that can be encountered during the sampling campaign.

Anthropogenic climate change is altering marine ecosystems not only at an unprecedented rate, but also in ways that push these systems outside their natural range of variations (IPCC Report, 2014). In order to understand the impact of ocean warming, ocean acidification, and deoxygenation on marine ecosystems and global biogeochemical cycling, Earth System models are reliant on in situ and remote sensing observations in order (1) to calibrate and validate model results for the present and past period (observational constraints for modeled quantities, testing of different model versions, constraining poorly known processes and parameters, data assimilation); (2) to supply modelers with high-resolution, global-scale maps of relevant observables and ancillary information (e.g. marine biogeography or global scale pCO_2 distributions); and to (3) further develop models and test new concepts (e.g. the influence of mesoscale variability on ocean productivity and carbon uptake). Analogous studies in inland water environment are only making their first steps. It is known that in many lakes CDOM (that can be detected from space) is in good correlation with DOC comprising the main pool of carbon in lakes. It has been shown that DOC concentration in lakes is in correlation with pOC_2, meaning that estimating lake pOC_2 may be feasible.

Whereas the biological applications of ocean-colour products are increasingly understood, it is less widely-known that they have their uses in physical models of the ocean as well. Ocean-colour is used to provide boundary conditions in flux calculations: for example to prescribe light in the visible domain (~400 to 700 nm) reaching the water surface (see the session devoted to PAR at CLEO).

Also from a physical perspective, optical properties of waters, derived from ocean-colour data, are important in calculations of the profile of light penetration, and hence solar heating through the water column (the ESA TIE-OHF Project has a component that deals with this application of ocean colour products). In this context, one can think of phytoplankton and other particulate material in the ocean as “marine aerosols”. Just as one would not ignore atmospheric aerosols in calculations of transmission of solar radiation through the atmosphere, so also is it important to account for the role of particulate matter (phytoplankton and other material in suspension in the water) as well as coloured dissolved organic matter, when calculating light transmission and solar hearing through the upper layers of the ocean.

The discussions at CLEO also recognized the common and cross-cutting needs for ocean-colour products across many communities. Many of the requirements of marine and inland water environmental services from ocean-colour data are the same as climate requirements. Ocean colour is also recognised as an Essential Ocean Variable, which admits a broad range of applications, beyond climate. Within GOOS, its Biogeochemistry Panel takes responsibility for Ocean Colour. But GOOS recognizes the cross-cutting nature of ocean colour.

Recommendation: Common messages are important: GCOS/GOOS to work together with respect to commonalities in ocean colour as an Essential Climate Variable as well as an Essential Ocean Variable.

Recommendation: The workshop recognized the importance of exchange and transfer of products and information between environment and climate services (recognizing that this is already happening at many levels), to avoid duplication of efforts.

1.3 State of the Art

The presentations in the session on "Ocean-Colour Applications for Climate Studies" gave a broad idea of the state of the art. The invited talk by Brian Franz described the NASA activities. NASA carries out careful and sustained work on sensor calibration and stability, ensuring the quality of products from individual sensors, and ensuring inter-sensor consistency. The presentation by Meike Vogt highlighted the importance of using ocean-colour products, modelling approaches and in situ observations in an integrated manner, to arrive at a four-dimensional vision of ocean biogeochemical processes. Racault and colleagues highlighted the use of OC-CCI data to study regional impacts of ENSO-related climate variability on the marine ecosystems. Sammartino and colleagues presented a novel method to derive the vertical structure in chlorophyll in the sea, with inputs from ocean-colour data. Martinez and colleagues discussed algorithms for estimating phytoplankton carbon from space, their intercomparison and their evaluation using OC-CCI data and a newly-compiled in situ database. These oral presentations were complemented by a number of poster presentations that highlighted a variety of applications ocean-colour data for climate studies, including various modelling applications; the use of profiling floats for calibration of ocean-colour data; climate trends in coastal waters off Ghana and their impact on fish; the socio-economic impacts of intense macroalgal blooms off Chile; use of ocean-colour data to validate primary production models; contributions to biogeochemical studies of lakes; and atmospheric correction methods for turbid waters.

The participants recognized the advantages of ESA and NASA working in a coordinated manner on the generation of climate products. The OC-CCI project focuses on selection of best algorithms for climate studies (for both atmospheric correction and in-water products) generating an inter-sensor bias-corrected time series of products that incorporate multiple missions and are uncertainty-characterized and validated using in situ data. It is important for the user community to know what exactly the Copernicus Climate Services will do in this regard.

Recommendation: The CLEO workshop recommends agency or inter-agency level consistency in processing chain for reprocessed products for environment and climate service users.

Recommendation: The participants appreciated the meticulous work carried out by the NASA Ocean Biology Processing Group to ensure the calibration and stability of the products generated by NASA for the individual ocean-colour missions, and to improve the compatibility between multiple missions. These approaches, complemented by OC-CCI work, should be seen as a blueprint for the effort required in deriving and maintaining climate data records for Ocean Colour.

Recommendation: ESA should continue to generate, maintain and update the OC-CCI time series data, working in close collaboration with EUMETSAT, NASA and with the Copernicus Climate Change Service.

Recently, a wide range of products capturing aspects of the biological carbon pump from remote sensing observations has been made available for the modelling community. The range of products comprises estimates of net primary production, phytoplankton carbon biomass, phytoplankton functional types, phytoplankton loss rates, suspended particulate organic carbon, particle size spectrum, and rates of export fluxes. Thus, a full quantification of the upper ocean biological carbon pump using remote sensing products seems no longer out of reach, and would be essential to better constrain marine ecosystem and climate models.

Large amount of dissolved and particulate carbon is contaeined in coastal waters. Although the optically complex coastal part is small compared to the whole global area of oceans, the concentrations of carbon are by orders of magnitude higher there than in open oceans and lots of carbon processing takes place there. On the other hand remote sensing products are not accurate (compared to oceans) in optically complex coastal waters and OLCI type 300 m spatial resolution is not sufficient in many geomorphologically complex coastal waters.

Recommendation: It is important to add to the product suite generated by OC-CCI. Products of special interest to the user community include primary production and export production, light at the sea surface, pools of carbon in the ocean, phytoplankton phenology and phytoplankton functional types. Note: Most of these applications of ocean-colour data were also discussed during other sessions at CLEO.

Recommendation: The launch of Sentinel-2 opened completely new possibilities in lake and coastal carbon studies. Radiometric resolution of the MSI is sufficient for waterbodies and the spatial resolution is sufficient for all lakes, great majority of which are very small. ESA should use this technical advancement to make significant step forward in determining the role of lakes in the global carbon cycle.

1.4 Gap Analysis

The participants discussed issues associated with continuity and consolidation. The curation of ocean-colour data over the long-term (multiple decades) was recognized as being critical for detection of climate importance.

Recommendation: OC-CCI Initiative that provides long time series by careful merging of data from multiple missions should continue uninterruptedly. If not continued, it would lead to substantial weaknesses in our ability to use these data for climate research. The achieved consensus on fundamental principles on how the climate data records should be generated should be sustained and developed.

Recommendation: Time series should be protected from gaps in data stream (key to have two sensors in orbit at the same time). Sentinel-3 mission, with the promise of 2 sensors with high spectral resolution in orbit at the same time in operational mode is an important beginning for climate observations, and should be continued for multiple decades, as planned.

Recommendation: Periodic reprocessing of the entire time series, in response to the addition of new sensors and to take into account scientific advances, is a necessity, to ensure that the products remain state-of-the-art as well as current. Reprocessing needs to be accompanied by careful and standardized analysis of the changes resulting from the improved processing.

Recommendation: Climate products should be generated with uncertainty characterization, to enable better interpretation of data, as well as the use of products in models, especially in data-assimilation mode.

Recommendation: Consistency should be maintained over the entire time series, to facilitate climate studies. Consistency within single products and across products should be maintained.

Recommendation: The provision of a great service comes with responsibility: it would be unwise not to spend a small fraction of mission budget on high-quality climate products and their access (user-friendly portals, user support, tool boxes). Such support services are important to facilitate user engagement and retention, as well as to avoid misuse of data. Gaps in such support services should also be avoided.

The participants discussed actions that might be undertaken to continue to improve the validation of products, and to improve the accuracy of products. Climate products must have a high level of accuracy, to be able to detect long-term trends in the data, which might be very small, and superimposed on high natural variability. The group felt that there were often too few in situ data to assess the validity of some climate-relevant ocean-colour products, for example, on the distribution of phytoplankton functional types. Merged ocean-colour products require a concurrent effort to maintain a select set of long-term oceanic time series for product validation, as reference stations. Validation programmes, such as the use of the Atlantic Meridional Transect (AMT) as a validation platform for Sentinel Missions is very important, as is the use of reliable new tools to improve the quality of validation data. Users are often not ocean colour experts, and require confidence in the products before they will use them. As such it is up to the provider to adequately vet and continuously check the validity of the products. Another point that was raised was the need for the validation exercises to incorporate an extended set of observations to enable testing and validation of novel products that are emerging. A particular example that was highlighted was the need to validate, and if possible improve, the calculation of photosynthesis-irradiance parameters from space, which was presented at the workshop.

Recommendation: The workshop recommended an integrated approach: It is important to bring together in situ observations, satellite data and models to study oceanic processes relevant in the climate context, to arrive at four-dimensional products. The products targeted should be related to Essential Climate Variables and Essential Ocean Variables as a first priority, and products related to ocean productivity and export, as well as plankton biogeography.

Recommendation: Consider data from autonomous and remotely-operated vehicles (e.g., gliders, bio-Argo) to add to validation data.

Recommendation: As the range of ocean-colour products for climate research grows, it is important that the in situ and validation programmes keep pace with the enhanced product line. (e.g., photosynthesis-irradiance parameters, see ESA's Project on Marine Primary Production Parameters from Space).

Recommendation: The participants pointed out that not many studies had made use of ocean-colour data to study climate impact. This was recognized as a missed opportunity that needed to be redressed. Hotspots of rapid change should be targeted for quick and important results. Such areas include the Arctic with retreating ice cover, coastal belts and areas of river influx. Such studies would add visibility and inform scientific debate.

Numerical biogeochemical and ecosystem models are one of the user communities of ocean-colour products. Such models are often interested in the carbon cycle, and usually represent phytoplankton and zooplankton in terms of their carbon content. This leads to a disconnect between what ocean-colour products provide typically (e.g., the most commonly used product is Chl-a) and what modellers specifically need. The participants recognised the strong effort from the ocean-colour community to take the step towards providing carbon products. At the same time, many ecosystem models now include dynamic Chl:C for the modelled phytoplankton. Consideration of physiological models and our understanding of the factors that underlie variability in the carbon-to-chlorophyll ratio could guide further developments in the retrieval of phytoplankton carbon products from ocean-colour data. On the other hand, satellite observations may lead to re-examination of models. Dialogue between ocean-colour and modelling communities are to be encouraged (e.g., POCO project).

Recommendation: A strong dialogue between ocean colour community and modellers would facilitate an agreed-on standard for use of ocean-colour products. Tutorials to target modelling audiences, workshops to agree on standards, documentation that do not rely on ocean-colour jargon are some of the possible ways to facilitate better co-operation between modellers and satellite oceanographers. Note: The Tech Notes provided with each OBS4MIPS product (see https://www.earthsystemcog.org/search/obs4mips/?template=obs4mips&limit=200) are examples of such documentation provided by the observing community for the modelling community.

At the same time, numerical models are now beginning to include output that relate more directly to ocean colour products. Given that the models do not have issues of missing data (clouds, satellite repeat cycles etc), and have 3-dimensional information, they could be useful laboratories to explore uncertainties in ocean colour products and help in the development of new algorithms. Even without these directly links to ocean-colour products, models can, and have been, used to provide information to the ocean-colour community (e.g. models have been used to provide estimates of the length of time series data needed before definite anthropogenic driven trends in Chl-a could be detected). The continued and improve use of models in helping address ocean-colour issues will require good communication between modellers and ocean-colour community.

Recommendation: Targeted workshops and funding opportunities to promote collaboration between modellers and satellite oceanographers is urgently needed to advance this promising direction.

1.5 Research and Development Priorities

The participants discussed actions needed to improve the contributions to IPCC reports based on ocean-colour products. The group recognized that, in spite of the relevance of ocean-colour as an ECV, there was an important gap in the use of ocean-colour data to study impact (or lack thereof) of climate change (or climate variability) on the marine ecosystems. In this connection, the group felt that some targeted regional studies might be undertaken to address this gap.

Recommendation: Development of targeted regional indictors: undertake case studies to illustrate the value of ocean colour as an ECV, to study variability and trends in biological and biogeochemical fields on a regional basis (e.g., small island states, the Arctic).

Recommendation: Using ocean-colour data with in situ observing systems to generate sub-surface fields with the adequate uncertainty estimation would contribute to studies of carbon export and other fluxes and the use of the prescribed fields in physics-only models.

Recommendation: Research and development should continue to improve algorithms to reduce uncertainties in climate products.

Recommendation: Improved algorithms for identification of phytoplankton functional types or species are a priority. These activities should bear in mind that different remote-sensing approaches exist to study PFTs, and that they target different aspects of the problem. Complementarity with modelling approaches should also be recognized and used to provide auxiliary information.

Recommendation: In light of the recommendations above, hyperspectral missions should be considered, in addition to multi-spectral (e.g. Sentinel-3) type of missions. The missions should take into consideration the temporal and spatial scales of relevance to studies of phytoplankton.

Recommendation: Use of ocean colour in studies of both, ocean and inland water carbon pools (dissolved and particulate, organic and inorganic) and carbon fluxes (primary production, export production, land-sea fluxes and air-sea fluxes) should be encouraged, as a means to close the global carbon budget. Novel applications, such as using ocean-colour data to derive parameters of primary-production models, are to be developed further, for use in climate studies. Their importance lies in their contribution to understanding how photosynthetic rates in the ocean might respond to changes in the marine environmental properties, such as temperature, light and nutrients.

Recommendation: The use of ocean colour in radiation budget studies (e.g., PAR and its spectral constituents; penetration of solar radiation into the ocean) should be developed further.

Recommendation: The participants recommended that the use of Lidar data to improve ocean-colour products in marginal ice zones be explored. The use of Lidar in combination with passive instrument in general should be considered, for example to provide information on the vertical structure of phytoplankton communities. Examples exist of deployment on aircraft that has provided some first glimpse of what can be achieved using Lidar for detection of phytoplankton communities.

Recommendation: Development of cross-sectorial linkages, such as the use of ocean colour to study marine ecosystems; use of ocean-colour to study socio-economic impacts of ecosystem variability, harmful algal blooms; and fisheries applications should be treated as priority.

Recommendation: Transfer of information from science policy makers as evidence base for decision making is another important area that requires further attention. The use of ocean-colour in discussions about geo-engineering should be encouraged. It is important to recognize the broader context within which climate considerations operate. Climate effects never manifest themselves in isolation from other environmental factors. It is therefore an integrated approach that is most likely to be effective.

Session 2: Light Field in the Ocean: Primary Production and Ocean Dynamics

Emmanuel Boss, Didier Ramon, Robert Frouin, Dominique Jolivet, Shubha Sathyendranath, Heather Bouman, Thomas Jackson.

2.1 Introduction

This report provides a scientific roadmap for the uses of, and priorities for the development of radiant flux products at the sea surface and in the interior of the ocean. Various applications of photosynthetically available radiation (PAR) data, including in the fields of primary production and ocean dynamics emerged from presentations (oral and poster) during the dedicated session at the CLEO workshop at ESRIN on 6-8 September, 2016, and the corresponding discussion session. The discussion session began with the following seed questions:

- Do existing PAR and shortwave downward flux products meet the requirements of the global climate, atmospheric, oceanographic and biogeochemical communities? What can be done to serve better the needs of the user community in general and the modelling community in particular?
- What additional products should be added to the product streams to increase their usefulness? What should be the characteristics of these products in terms of temporal, spatial and spectral resolution, spectral range, and accuracy?
- What are the needs in terms of harmonization between sensors, methodologies, ancillary data and radiative transfer tools?

2.2 Why do Radiation Fields Need to be Quantified for the Upper Ocean?

The following application domains were identified:

- Biology

Solar radiation in the photosynthetically active range (roughly 400-700 nm) controls the growth of aquatic algae. It ultimately regulates the composition and evolution of marine ecosystems. In addition, ultraviolet (UV, 280 – 400 nm) light has the potential to stress phytoplankton and inhibit primary production.

- Chemistry

Solar radiation in the UV interacts with dissolved organic molecules to produce a variety of products including peroxides. In the process, it reduces the absorption by coloured dissolved organic matter (CDOM), increasing light penetration.

- Physics

Absorbed short-wave radiation heats the upper ocean affecting mixed-layer dynamics and oceanic circulation. This absorption is modulated by the in-water constituents, including phytoplankton, and hence involves cross-disciplinary processes, including biophysical feedbacks. Solar heating in turn influences air-sea exchange of heat, atmospheric temperature and circulation. Solar radiation reflected by the ocean affects the outgoing radiative flux from the planet (planetary albedo), with climate consequences.

2.3 State of the Art

Only a few apparent optical properties are presently inferred reliably and operationally from space, namely spectral reflectance, downwelling planar irradiance just above the surface integrated from 400-700nm ('daily PAR product'), diffuse attenuation coefficient at 490 nm and planar spectral UV irradiance at noon. These products are derived for each ocean-colour mission individually (notice that UV sensors are not available on standard OCR missions).

Existing satellite products generally do not cover the entire global open oceans (e.g., retrievals limited to Sun zenith angles < 75 deg.), and they do not provide information below sea ice. In addition, cloud diurnal variability is not accounted for in daily PAR calculations when using polar orbiting satellites. Propagation of surface radiation to depth often assumes that the upper ocean is homogenous, neglecting potentially important effects of stratification on the absorption of radiation.

2.4 User Needs

User needs are variable in terms of products, spectral, spatial, and temporal resolution and acceptable uncertainties.

The participants recommended that the products should be easily accessible, should have associated detailed protocols including description of all ancillary data used and their sources. Computer codes used to derive products should be available to users.

For certain applications (e.g. associated with climate), products need to be sensor independent, consistent and continuous across satellite missions.

In addition to currently produced and distributed solar irradiance products, there is a need from the community (based on recent PML survey) for:

- Sub-surface planar and scalar irradiance (as opposed to above the surface)
- Fraction of PAR absorbed by phytoplankton (APAR)

- Diffuse fraction of total irradiance (average cosine of light field just below the surface).
- Spectral planar and scalar irradiance.
- Surface albedo (ratio of planar upwelling irradiance to downwelling planar irradiance just above the ocean surface).
- UV-A, UV-B scalar irradiance (with photon and energy units).
- Sub-surface light fields.
- Products without gaps (in space/time) to provide boundary conditions to models.
- Upper-ocean heating profile.
- Diurnal distribution of PAR and its attenuation.
- Averaged mixed-layer PAR.
- Under-ice light fields.

2.5 Gap Analysis

Some products (such as below surface PAR) can be easily implemented while some others require development. The state-of-the-art is such that the strategy to obtain the new products described above is known summarized in Table 1.

Spectral fields should be provided at the sensor resolution with protocols (and codes) describing how to interpolate and extrapolate to obtain other spectral distributions (e.g. 5nm irradiance field from a multi-spectral sensor).

Vertical propagation of products requires an appropriate attenuation coefficient from which other products can be derived (e.g. euphotic depth, isolume depth). Clear guidelines on how to produce the derived products using the attenuation should be provided.

Horizontal/temporal gap-filling is necessary for certain applications. This can be done using merged products across sensors and/or interpolation schemes (using known de-correlation scales or models).

Products should have realistic associated uncertainties that have been validated with in-situ data. This requires a cal/val program. The product protocol should provide a description of how the uncertainty was derived. It is desirable to provide a per-pixel uncertainty. It is recognized that the level of effort to obtain a very accurate uncertainty estimate can be very large and therefore some trade-offs may need to be done, in consultation with user requirements.

Data access should be tailored to users need. For example, modelers will use THREDDS and will need simultaneous access to associated error fields. In contrast, the EO community will, typically, want to access data using FTP. Most users do not care about the mission from which a product was derived, but rather care about the products being continuous in time and consistent across missions.

Table 1: New radiation field Products required by users and their technological readiness.

Products	**Definition**	**Possible methodology. Difficulties/Opportunities**	**Readiness level**
$E_d(0-, \square_i)$, $E_o(0-, \square_i)$	Sub-surface planar and scalar irradiance (as opposed to above the surface) at satellite sensor bands	Sub surface downward irradiance is a direct product. Scalar irradiance is just another output of the algorithm that yields planar irradiance from the satellite radiance measurement	High
$s<\mu\ >(0-, \square_i)$	Diffuse fraction of total irradiance above the surface or average cosine of downwelling light field just below the surface	The directional dependence of the downwelling light field above surface, apart from the solar zenith angle, is controlled mainly by cloudiness. It can be parameterised, which requires some modelling effort. It can be propagated to just below the surface without difficulties knowing the sea surface state and applying Fresnel's laws.	High
$E_o(\lambda)$	Spectral scalar irradiance (with photon and energy units).	If the satellite is measuring at the wavelengths of interest, it is easy in the visible and NIR though not demonstrated yet in the UV. Otherwise there is a need of a clear sky and cloudy sky model for spectral extrapolation or interpolation. This has to be studied case by case. In the visible range outside atmospheric strong absorption bands, there is	High to moderate depending on wavelength range

		no major difficulties for such a model. There is a specific need for UV-A and UV-B spectral range which controls several photochemical processes. The strong atmospheric absorption is an issue especially when the coupling to scattering is important with high aerosol loading or cloudy sky	
A(λ)	Surface albedo (ratio of planar upwelling irradiance to downwelling planar irradiance just above the ocean surface)	This is limited to clear sky pixels. There is a need to introduce a BRDF model of the ocean. The glint part comes from the wind speed and wave model like Cox & Munk's (1954), the water BRDF should be parametrized from spectral remote sensing reflectance.	High
PAR(t)	Diurnal distribution of PAR.	Instantaneous PAR is a common product. Its diurnal variation can be measured from space using geostationary satellites, Lagrange L1 point located sensors or with sun-synchronous LEO constellations with a range of overpass time spread along the day. From a unique LEO sensor, ancillary data about the diurnal variation of cloudiness is necessary.	High
$K_{d\_PAR}(z)$	Vertical attenuation of PAR	Estimating the vertical attenuation of PAR in the water column requires knowledge of water reflectances, and thus is restricted to clear sky	High/Moderate

		pixel. Alternatively, attenuation within the water column, in clear and cloudy conditions, could be sensed by lidar	
Mixed Layer PAR, PAR at the bottom, PAR(z)		Computed from MLD (assimilating model input), PAR(t) and <Kd_PAR>	High/Moderate
APAR	Absorbed fraction of PAR by algae	Need the phytoplankton spectral absorption. Alternatively APAR can be derived directly from spectral water reflectance	Moderate
h(z)	Upper-ocean heating rate profile.	Need the vertical profile of the spectral absorption coefficient	Moderate
Under ice fields	All quantities under ice	Need an ice-sheet snow transmission model	Low

Recommendation: Cross-agency efforts should be made to homogenise their respective products so it is easy for users to use these products (e.g. the definition of PAR product should be the same). For climate relevant products, it is critical to merge them (and de-bias) across missions so that models to not experience secular jumps as they assimilate such data.

2.6 Research and Development Priorities

2.6.1 Short term

Recommendation: Some user needs can be addressed by previous, present and future sensors, and the immediate action should be on Level 2 and Level 3 processing. For example, the SEOM project PAR for Primary Production addresses several needs. New processing lines require links with other Ocean and Atmospheric products and/or ancillary data (ex: Met reanalysis). An issue is which MLD definition is most appropriate for NPP calculations (there are many definitions).

Recommendation: With existing knowledge, derive the following products from current and past missions (see Table 1):

- E_d(0-), E_o(0-), <μ>(0-), E_o(λ) for Visible-NIR, PAR(t), K_d_PAR, A(λ), APAR

Recommendation: A cal/val program should be planned to evaluate the new products and their accuracy over a representative set of conditions.

2.6.2 Medium–term (longer–term effort not lower priority)

Recommendation: With specific effort in algorithm developments, derive the following products for future, current and past missions:

- E_o(λ) for UV-A, UV-B (with photon and energy units) in conjunction with Sentinel 5/5P.
- Averaged mixed-layer PAR (in conjunction with Mixed Layer Depth fields from Argo-assimilated circulation models).
- Products without gaps (in space/time) to provide boundary conditions to models.
- Upper-ocean heating profile.
- Under-ice light fields (in conjunction with cryospheric missions and modelling).

Recommendation: As for 6.1, cal/val activities should be organized to evaluate the new products and their accuracy over a representative set of conditions.

2.6.3 Future vision

Recommendation: For significant improvement of sub-surface light fields, space-lidars could be used (e.g. CNES' MESCAL) as they can resolve the vertical distribution of material in the ocean (while all the products described above assume a homogeneous upper ocean). This is particularly critical in high latitude regions (near the ice) and near land.

Recommendation: For significant improvement in daily-integrated radiance fields (e.g. due to clouds), diurnal-cycle resolving measurements, combining different satellite, over-passing at different times, with geostationary satellites, should be pursued.

Recommendation: Use of highly resolved spectral sensor that can resolve Fraunhofer lines to provide the two-way light attenuation at specific bands (proof of concept shown by Dinter et al with OMI).

Recommendation: Satellites missions with instruments in L1 orbit (e.g. NASA's DISCOVR) will offer the opportunity to continuously observe the sun-lit part of the ocean, maximizing the temporal coverage. Space agencies should explore using such orbit for an Ocean Color satellite mission.

Session 3: Turbid waters and highly absorbing waters

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3.1 Introduction

The first satellite ocean colour data in the early 1980s established that phytoplankton can be detected in the open oceans and the first ocean colour algorithms focused on chlorophyll estimation for these “case 1” waters. Since then, with the rapid improvements in the spectral, spatial and radiometric performance of satellite hardware, many new applications have emerged, particularly in coastal and inland waters where human impacts are often most severe. These new applications require the development of data processing algorithms both for atmospheric correction and the estimation of water properties, such as chlorophyll and suspended particulate matter concentration, and these algorithms must function in waters that are considered more and more “extreme” in terms of scattering and/or absorption coefficient.

State-of-the-art, new developments as well as gaps and needs for further scientific and technological developments were discussed at the during the session “Turbid Waters and Highly Absorbing Waters” and the corresponding Discussion Session at the CLEO workshop at ESRIN on 6-8 September, 2016, organised by the ESA SEOM Case2Extreme Project. The discussion session was structured along the following seed questions:

- Case2 and case2extreme waters: coastal and inland – where are the differences, what is in common (algorithms, validation, pre-processing, derived products)?
- What new products for extreme Case 2 waters can be expected using OLCI, SLSTR and Sentinel 2 MSI?
- Where are the limitations of algorithms for water constituents and how can we stretch these limits?
- Uncertainties – What kind of information on product uncertainties do users need, and are we able to generate it? How can we validate the uncertainties?
- How does OLCI fit within the other missions? (is there a huge discontinuity of RS data, a shift in products between sensors…)?

This report provides a draft for a scientific roadmap for the further development and use ocean-colour products in turbid and highly absorbing waters, as typically found in coastal areas, inland waters, and which are traditionally referred to as Case-2 waters.

3.2 Requirements

In his talk “Requirements for ocean colour observations and products in turbid and highly absorbing waters”, Mark Dowell from the European Commission presented an overview of the large diversity of applications which are lacking information and which benefit from ocean colour measurements. This list includes, among others, climate change, ecosystem state, carbon cycling, water quality, benthic habitat mapping, fisheries support and management, HABs, aquaculture, sediment dynamics, dredging, marine spatial planning, eutrophication monitoring, conservation and biodiversity, to name just a few key applications. The second key note talk by Kevin Ruddick had shown that ocean colour observations of (extreme) Case 2 waters can provide parameters supporting these applications, such as chlorophyll-a concentration, total suspended matter concentration, turbidity, CDOM absorption or diffuse attenuation coefficient. The following high level topics have been identified in the discussion session which pose requirements for further improving product quality and/or generation of new products better serving coastal applications:

- Atmospheric correction
- Optical Water Type (OWT) classification and algorithm selection, especially with respect to a typification of water bodies for Water Framework Directive reporting
- Characterisation of the specific optical properties (SIOPs) of water bodies by in-situ measurements
- Uncertainties
- Chlorophyll-a and CDOM retrieval improvements
- Carbon related products
- “non-concentration” products, such as spatial pattern and surface features
- Masking of pixels (cloud and cloud shadow, floating vegetation, sea ice, …)
- Exploiting new technologies, such as drones, in combination with EO and in-situ data

3.2.1 Atmospheric Correction

The atmospheric correction (AC) has implication on all coastal and inland water products and has been identified by the group as still **the n°1 issue**. It is particularly challenged in the context of extreme coastal and inland waters. Users need accurate AC (optimal decoupling between ocean and atmosphere), uncertainty estimation, proper masking (identification of pixels not suitable for atmospheric correction, i.e. at input, as well as flagging pixels with unreliable atmospheric correction, i.e. at output). Users further require maximum spatial and temporal coverage, i.e. an atmospheric correction that works under very many different conditions.

3.2.2 Optical Water Type and Water Framework Classification

The EU (European Union) Water Framework Directive (WFD, Ferreira et al., 2007) concerns most of the water areas identified as some type of C2X-waters, being mostly coastal and lake water environments. Therefore, user needs for Case 2 extreme waters mostly arise from WFD perspective if the application is among monitoring obligations. WDF reporting requires assessing the status of coastal and inland waters using water bodies as classification units with sufficient confidence and precision through the directive's monitoring programs. The major interest in WFD requirements concentrate on the accuracy of defining the chl-a concentrations near good/moderate. If a water body is assigned to moderate class (or worse than moderate), it sets requirements for improving the status of the water body. Therefore, the accuracy requirements set for EO products are highest near this class limit. For WFD classification, the reference conditions and class boundaries are defined for each water type. The reliable establishment of classification relies on type-specific reference conditions. Water types are defined based on pre-knowledge of the water body. For example, in Finland, the amount of CDOM in water body is important part of water body typing, as part of the lakes and coastal areas, especially estuaries are extremely humic. The CDOM dominated waters have different class limits for chl-a classification than non-humic water bodies. Thus, the importance of defining the level of humic substances for water bodies is high. The amount of humus in water body increases the uncertainty of EO derived chl-a, thus it is relevant to account in optical typing of the water bodies.

Quality classification case example for WFD: During the CLEO discussions, the need to define a quality classification map to separate the regions where EO products already have sufficient accuracy from those that still need algorithm development was identified to fulfil the user needs. This would serve as a practical tool for communications with the user and to increase the credibility of the EO products.

As a case example of this, a recent quality classification of MERIS chl-a products was conducted for 215 coastal water bodies (Attila et al. 2016 *). A quality classification method was applied to determine the accuracy of MERIS- derived chl- a at coastal sites and water bodies, where chl- a data derived from MERIS can be biased by the presence of other substances besides phytoplankton, such as SPM and CDOM and can also be influenced by bottom reflection. For this, information on the size of water body, average water depth and routine monitoring station measurements of Secchi depth (ZSD), turbidity and Pt water color (as an indicator of humic material) were utilized. As a summary: 87% of the surface water areas covered by WFD water bodies in Finnish coastal waters can be estimated reliably using chl- a derived from

MERIS. This accounted to 44.2% of the studied coastal water bodies. 40.5% of the remaining water bodies could be estimated during most of the periods, excluding periods of high river run- off occurring after heavy rains and snow melt during spring. During these periods, the amounts of SPM and CDOM increase temporally, affecting the retrieval of chl- a. Chl- a estimation thus still need to be improved for the small inner water bodies that are affected by high loads of run- off, e.g. close to estuaries. In total, these areas account, however, for less than 10% of the case example surface water area in Finnish coastal waters (Attila et al. (2016*). The work will continue with Sentinel data (S2 and S3) and water bodies on lakes.

For S2/MSI instrument, we foresee that the bottom effect needs to be accounted in more detail. Nevertheless, it will also increase the amount of WFD water bodies with better EO quality class due to its ability to capture small inner water bodies. S3/OLCI instruments, we foresee that there will be improvement in algorithm development, especially for separating the different components of absorption and thus the quality classification accomplished for MERIS is likely to improve with OLCI era.

3.2.3 Water Characterisation

In situ measurements of concentrations and SIOP are crucial for development, calibration and validation of EO algorithms. These are also directly used in the assessment of the quality/status of coastal & inland waters, as part of the WFD, MSFD. For Case2X waters the amount of high quality in situ data (matchups) available to the EO community is still low and lack harmonization. These shortcomings are due to:

- Use of different instruments and protocols (e.g. use HPLC, Fluorometry, or spectrophotometry for Chl-a or cleaning interval of continuously measuring devices)
- Technical limitations of instruments for light field measurement in C2X (e.g. saturation, inaccuracy)
- Use of different data processing methods and quality control (e.g. the accuracy of sky reflection removal in above water Rrs measurements esp. in C2AX)

Why do we need to optically characterize water?

- Crucial to calibrate and validate RS algorithms, to provide L2 products (also for ecosystem or sediment transport models, carbon cycle studies, etc.)
- which help assess quality/status of coastal & inland waters, as part of the WFD, MSFD
- Can support water types classification (or validation of WT classification tools)
- Large database of SIOPs, IOPs for Case1 waters, but little exists for Case2X waters

3.2.4 Masking of Pixels

The objective of the pixel masking is the identification of invalid and insufficient pixels in order to provide users products that 1) are reliable with respect to the subsequent AC, 2) provide consistent time series, 3) retrieve valid products used for reporting and analyses.
This concerns both - pixels where obvious conditions hinder algorithms to work (clouds, cloud shadows) as well as pixels where algorithms do not work properly (training ranges and limits, shortcomings of algorithms). In the end the products should be free of artefacts (cloud border, shadow effects). Users are algorithm developers, scientists to analyse data and processes, service providers and finally users that need information for reporting.

3.2.5 Chlorophyll–a and CDOM retrieval

It was noted earlier that Chlorophyll-a concentration is the most widely used indicator for WFD assessment. However, in areas influenced by humic substances and CDOM (boreal and Arctic lakes around the world, Baltic Sea) is the key factor determining the colour of water. Consequently, it is an indicator on water quality directly, and used for for trend analysis (brownification), and in CDOM dominated eutrophic waters hard to estimate chlorophyll-a without knowing the CDOM concentration precisely.

3.2.6 Carbon related products

The need to know the carbon cycle in the open ocean for climate modelling, is well accepted. Lakes are sentinels and regulators of climate change and play and important role in the global carbon cycle (Tranvik et al. 2009, IPCC 2014). More than 90% of carbon in lakes is in the form of dissolved organic carbon (DOC), part of which is coloured (CDOM). Knowing the DOC content in lakes is not crucial only for global carbon cycle studies, but also in drinking water treatment where the DOC has to be removed and variable amount of DOC determines the amount of chemicals that has to be used. Particulate organic carbon (POC), particulate inorganic carbon (PIC), and dissolved inorganic carbon (DIC) are also important carbon constituents and its estimation from remote sensing data has been shown. There was a whole discussion session on carbon pools in the ocean, and most of the topics discussed there are applicable for (extreme) Case 2 waters, too.

3.2.7 Non–concentration Products

The optimal scenario would be to provide end users with high accuracy absolute level products. This would, for several processing steps and products, require further R&D work. However, existing methodologies can, in many water types, provide information on a

relative scale that would be sufficient in order to support many end user needs.
European end users are focusing their efforts and limited funding to respond to the requirements of the European directives WFD, MSFD, as already explained. Several parameters and indicators need to be measured and estimated in order to assess the ecological status of all water bodies >0.5 km^2. Rather than directly providing concentrations of some of the include parameters, e.g. chl a, EO could provide relative distribution maps as input to modelling actions relate to several factors included in the directives, e.g. probability of presence and level of abundance of benthos, macrophytes and fish. Time series indicating fluctuations in the level of organic matter could support increase or recovery from acidification. This type of products can also support water managers in planning in situ sampling activities as not all water bodies can be covered and stratified and rotating sampling schemes will be necessary.

3.2.8 Uncertainties

Estimation and communication of measurement uncertainties is important for building trust in EO products, for correct comparative analyses with other measurements (e.g. for validation) as well as indispensable input for model assimilation. Uncertainties themselves need to be validated. Currently there is no agreed protocol for uncertainty estimations or their validation.

3.2.9 New Technologies

(Extreme) Case 2 waters pose demanding requirements on space borne optical instruments. They exhibit large variability in terms of both, spectral shape and amplitude, across a wide spectral range from UV to SWIR. However, this also offer possibilities for exploiting the signal, e.g. in future instruments. A non-comprehensive list is provided below:

- Spectral range of Instruments to improve AC:
  - Highly absorbing waters need measurements in UV
  - Highly scattering water need SWIR
- Cloud detection over bright waters need more cloud specific bands (SWIR/NIR)
- Multi angle observation to improve aerosol characterization
- Polarized observation to improve aerosol characterization, in particular to separate surface and atmosphere
- Higher number of bands to reduce ambiguity / similarity, when disentangling of contribution of water and atmospheric constituents
- Radiometric characteristics of Instruments to improve AC and retrieval of water constituents:
  - Highly absorbing water may require very high gain with very low noise

    - SWIR signal have less solar signal and thus requiring higher sensitivity
    - Very low radiometric noise to reduce the shielding effect of instrumental effects
- High spatial resolution:
    - C2x water often belong to small scale features
- C2X waters require demanding inversion procedures:
    - Using full spectral resolution procedures to disentangle of contribution of water and atmospheric constituents (instead of simpler band ratios/differences)
    - Using 'complete inversions' (not discriminating between atmospheric correction and water body inversion)
    - Assimilation techniques to reduce the ambiguity by adding additional knowledge (vertical profile of water constituents, time/location specific spectra of absorption and scattering water constituents)
    - Floating and subsurface algae detection
- C2X waters require demanding validation procedures:
    - C2X water characteristics are probably highly variable. AC and Inversion techniques working on one site/season do not necessarily work on other sites. Thus a validation for one site may not be valid for other sites.
    - Parallel LIDAR measurements, may allow instantaneous verification (B_b profile up to optical thickness of 3)
    - New measurement devices for in situ (in particular scattering properties) will be needed
- C2X waters require demanding radiative transfer modeling
- In situ optical measurements equipment is designed for clear ocean waters and cannot be used even in conditions that are far from extreme

In addition to the new technologies driving improvements in space hardware, we expect new technologies to lead to improvements in capabilities for in situ measurements to support and/or validate the satellite data products. Key technologies there are: the massive improvements in wireless data communication facilitating the networking of instruments; the miniaturisation of electronics and associated reductions in power requirements, and; improvements in optoelectonics used in radiometers, imaging systems, scattering and absorption meters, flow cytometers, and fluorimeters allowing more and better measurements to be made of optical parameters, including the Ultraviolet (350-400nm) and Near Infrared (700-900nm) spectral regions, potentially at very high spectral resolution, e.g. 1nm.

3.3 State of the Art

The presentations in the session on "Turbid waters and highly absorbing waters" highlighted the state of the art. A good overview was included in the key-note talk by Kevin Ruddick which benefitted from the results of the ESA Case 2 Extreme project. In summary, critical issues such as proper characterisation of the large variety of water bodies in optical terms, the atmospheric correction, inversion methods and validation, have been clearly identified and good progress has been achieved. Atmospheric correction improved compared to few years ago. Products related to backscatter can be retrieved with good quality while absorption related products, namely Chlorophyll and CDOM, are still very challenging. Optical water type classification is an evolving subject where good initial results are available.

3.3.1 Atmospheric Correction

Today three different types of atmospheric correction (AC) algorithms are available, at different levels of maturity and applicability in extreme Case 2 waters:

Extrapolating AC is well studied in Case 1 waters. However, it is challenged in scattering waters by increased signal in the NIR. There extrapolation errors lead to over-estimation of atmospheric component, to some extent mitigated by iterative techniques. There is a clear benefit from the addition of SWIR bands for turbid waters processing, as available, e.g., in Sentinel 2 or by synergistic use of OLCI and SLSTR. This type of ACs is also challenged in absorbing waters by the low signal in the blue and often even in the green part of spectrum. Extrapolation uncertainty is leading to negative reflectances in the blue. These ACs are also known to be sensitive to sun glint, adjacency effect, and absorbing aerosols. The errors are mainly driven by the signal in the NIR/SWIR range.

Full-spectrum AC algorithms (e.g. C2RCC, Polymer) are far less sensitive to atmospheric perturbations. In particular there is no amplification of errors in the NIR/SWIR to the VIS range. They are physically based and rely on a water reflectance model. Beside the benefits from this, it poses also a limitation as the error of the AC increases where the water model does not reflect the real situation. The errors are driven by inaccurate modelling of the atmosphere or ocean.

Water-type specific AC, or ACs making assumption on local atmospheric variability are a new emerging field.

System Vicarious Calibration is applied to all types of ACs currently. However, SVC coefficients are derived under ideal, clear sky ocean conditions and applicability to coastal areas is still under investigation. Adjacency effect correction is not systematically applied in coastal AC.

3.3.2 Optical Water Types

Water bodies can be classified according to many different aspects and purposes, such as ecology, biodiversity, physical properties, or for the purpose of reporting for the WFD. Among the physical properties the optical water type classification is a technology in remote sensing to classify a water pixel according to its spectral characteristics, i.e. its colour. This method has evolved significantly in recent years as a tool to serve either the purpose of selecting most appropriate processing algorithms or ecological characterization. The different developments have been made for specific application and sensors without the ambition for a general, mathematically stringently elaborated method, in particular with respect to the link to atmospheric correction or to the application in merging algorithms.

3.3.3 Water Characterisation

The instruments used to optically characterise waters have been developed for open ocean or coastal waters and reach its limits when deployed in extreme conditions. They reach capability limitations: Case2SX (saturation), Case2AX (uncertainty) with increased inaccuracy as a consequence. Further, different instrument specifications may lead to e.g. discrepancies in time series. Measurement protocols also are available but are lacking adaptation to extreme optical conditions: above water reflectance (Rrs) experience weak signal in C2AX with related high uncertainties, the Fresnel correction especially in C2AX waters requires special attention. Below water reflectance (rrs) is also characterised by a weak signal in C2AX that may be negligible even below 650 nm as was shown by Tiit Kutser in his presentation. At the level of IOPs saturation of a, bb measurements can happen in C2SX and C2AX waters, respectively. There is a possible problem with the sigma-correction that needs attention. More attention needs to be put on measurements of the Volume Scattering Function (VSF). In general, a better standardisation of protocols is required.
Vertical distribution of optically active substance can vary largely in space and time, and is hardly known today. A proper sampling strategy for vertical profiles of IOPs is missing. Such profiles should reach ~1/2 Secchi depth, especially in stratified waters.

3.3.4 Masking of Pixels

Different algorithms for masking pixels are available, combining different information derived from the spectrum and form auxiliary data. Features that describe clouds and other pixel properties are used and subsequently combined in decision trees, Bayesian, or Neural Nets.

3.3.5 Chlorophyll–a and CDOM products

A large number of Chl-a algorithms for Case 2, including extreme Case 2 waters, have been published in the literature. However, these are mainly based on empirical relationships between in-situ measured Chl and an algebraic expression on 1, 2 or 3 spectral bands. However, these are lacking general applicability. Physically based spectrum inversion methods have also been developed, or are under development, e.g. in the ESA Case2X project. CDOM retrieval has attained much less attention, but also here most published algorithms rely on local tuning of band ratio algorithms. A neural based approach is currently under development in the Case2X project.

3.3.6 Non–concentration Products

The advent of Landsat-8 and Sentinel-2 has triggered a lot of interest in non-concentration products, specifically those related to surface structures. These instruments combine for the first time high spatial resolution with proper spectral band setting and reasonable radiometric quality (from ocean colour point of view). Algorithms for exploiting such features systematically and/or operationally are not yet available.

3.3.7 Carbon related products

For case-1 waters, POC is dominated by phytoplankton while for coastal and especially inland waters DOC (and it's coloured component CDOM) is the main pool of carbon. Validated methods for retrieval of DOC exist, but there are no established methods for POC in coastal areas alhthough algorithms have been published for inland waters. There is long way to go in order to establish DOC, POC, PIC and DIC algorithms for coastal and inland waters.

3.3.8 Uncertainties

The GUM provides the baseline for best-practice characterisation of uncertainties. This has been adapted in the QA4EO guidelines to Earth Observation, and is directly applicable to ocean colour algorithms and products. However, these guidelines need to be implemented at the concrete instrument and processor. The current practice is far away from this goal. For example, the Sentinel 3 OLCI L1b product foresees per-pixel uncertainties for the whole spectrum measured, however, this currently an empty placeholder in the products. Likewise are very few examples available where Level 2 algorithm descriptions contain a complete error characterisation following GUM / QA4EO guidelines, not to mention per-pixel uncertainties in products.

3.3.9 New Technologies

Instruments exists or will come in near future, that cover some of needed instrument characteristics, namely:

- Polder, 3MI (EUMETSAT) for polarization and multi-angle atmospheric characterization. However, these data have to be consistently used for atmospheric correction, uncertainties due to temporal shifts and different observation geometry and different spatial resolution have to be taken into account.
- Coming EUMETSAT Geostationary MTG for multi angel, with high radiometric quality, and high temporal resolution

- Synergy data of OLCI and SLSTR can be used to improve AC over C2S water, using SWIR bands of SLSTR and the new 1020 nm band of OLCI

(Extreme) Case 2 waters require demanding inversion procedures to exploit current and future sensors:

- Using full spectral resolution procedures to disentangle of contribution of water and atmospheric constituents (instead of simple band ratios/differences), these exists and/or are under development
- Using 'complete inversions' (not discriminating between atmospheric correction and water body inversion), these exists and/or are under development
- Assimilation techniques to reduce the ambiguity by adding additional knowledge (vertical profile of water constituents, time/location specific spectra of absorption and scattering water constituents), these exists but require further development

It should also be pointed out that products retrieved for extreme Case 2 waters require demanding validation procedures:

- C2X water characteristics are probably highly variable. AC and Inversion techniques working on one site/season do not necessarily work on other sites. Thus a validation for one site may not be valid for other sites. Work is in progress here, but this is currently insufficient.
- Parallel LIDAR measurements may allow instantaneous verification (b_b profile up to optical thickness of 3), feasibility study is available from NASA 'OPAL'.
- Hyperspectral absorption measurement are available and reliable
- Hyperspectral AOP measurement (R_rs) are available and reliable

3.4 Gap analysis

The State of the Art description highlighted already some points where current situation is not satisfactory and where a description of the status cannot be done without pointing to the required – but not yet addressed – next step.

3.4.1 Atmospheric Correction

There are four major areas where improvements of atmospheric correction is required:

- Limits of existing ACs are not characterized well enough
- The new spectral bands need to be better exploited.
- No satisfactory solution to provide uncertainty to AC
- Access to in-situ data and analysis tools needs to be improved

3.4.2 Optical Water Types

Reporting for the WFD (and similar laws in other countries such as USA or Australia) is currently in an embryonic state; most countries acknowledge the potential and some countries use it for coastal waters. A wider penetration into the national implementation plans is hampered currently by low quality of chlorophyll and CDOM retrieval in (very) turbid and absorbing waters, and lack of methodology to determine the WFD water type. Also the availability of remote sensing data with require radiometric and spatial characteristics is currently not sufficient but it is expected that full operational availability of Sentinel 2 and 3 will improve this gap. However, the value of Sentinel 2 and Sentinel 3 for WFD reporting needs to be demonstrated.
The Optical Water Type classification is considered the next evolutionary step towards a unified processing for Case 2 waters as requested by users. Currently a systematic assessment and harmonization of the different Optical Water Type classification methods is missing, and needs to be undertaken in order to achieve applicability for ecological characterization as well as guidance for algorithm selection or blending. An unresolved problem is the inherent linkage of the QWT with the atmospheric correction. Also a rigorous mathematical framework and scientific justification for blending algorithms based on an OWT classification is missing.
WFD reporting for coastal and inland waters requires a spatial resolution of 100m or better. Currently all sensors do not provide the required combination of spectral bands, SNR and spatial resolution.
To accomplish a generic Optical Water Type classification, an obvious gap is related to the lack of coherent network of optical in situ measurements to support and validate the Water Type classification. The availability of measurements defining the optical properties of the water varies between the countries. E.g. in national monitoring programmes the absorption of CDOM (humus) is not always included. Also, the methods and the accuracy requirements for defining water quality parameters varies between the countries.

3.4.3 Water Characterisation

A fundamental gap is the missing broadness of water bodies (coastal and inland) properly characterised in terms of optical properties. Too few data of absorption, backscatter and even much less data of VSF are available, but are required to achieve the required global applicability of algorithms. Further, has already discussed in the state-of-the-art section, the current instruments are not build / not sufficiently well characterised for deployment in extreme waters. Sensitivity, saturation levels and calibration need adjustment. Stability of instruments should allow for measuring consistent long term time series, in agreement with the time frame of the Copernicus programme.
A second big gap in water characterisation are vertical profiles.

Data should be made available in open and free accessible database. The data should become openly available shortly after collection in order to foster algorithm development and validation. The Aeronet network and data sharing principles are a good example.

3.4.4 Masking of Pixels

A single solution for pixel identification that is correct for every purpose is not possible. Subsequent algorithms always have different requirements, e.g. one AC algorithm is taking care of glint correction or haze correction, others do not and need a dedicated flagging, accordingly. The current way of pixel identification is yes/no, but also "uncertainty" or "probability" flags are introduced (SURE, PROBABLY, UNLIKELY) as done for Landsat-8 and Sentinel-2.
The identification of non-water pixels is already working well for cloud detection and land/water separation, especially for the medium resolution sensors. The quality depends on the availability of bands (e.g. SWIR, thermal). And still, activity is going on to improve them. The challenge is to find globally applicable algorithms that work for diverse conditions (sun elevation, extreme turbid waters, optical thickness, glint, floating vegetation). New challenges arise with higher resolution images for water quality. The shadowing effect not only from clouds but also from constructions (wind mills, harbour constructions, surrounding mountains, identification of ship emissions) need to be taken into account more intensively. Shadow effects need the sun and viewing geometry and height of the objects, partly taken from the satellite themselves (thermal bands, O2 bands), but not given in all sensors.

3.4.5 Chlorophyll–a and CDOM products

Chlorophyll-a and CDOM algorithms still suffer from low accuracy in (extreme) Case 2 waters. In particular in highly absorbing waters a good separation of Chl absorption and CDOM absorption is to be achieved. One way to improve this is to better optically characterise waters, and extend this to as many water bodies as possible. These data then need to be included in the algorithm design and improvements.
The vertical distribution of optically active substances is always assumed well mixed. Stratification is not addressed.

3.4.6 Carbon related products

There are currently no solutions for optical complex waters to determine POC, PIC, and DIC. In inland water DOC contributes 90-95% of carbon in inland waters and thus focus should be on DOC.

3.4.7 Non–concentration products

Visual inspection of images, specifically Landsat-8 and Sentinel-2, demonstrate that spatial features can be detected in images and these are of interest for users (e.g. wind patter, surface pattern behind wind parks; dumping from ships, …). Algorithms to automatically extract these features and annotate them with certain metrics do not exist.

3.4.8 Uncertainties

Uncertainties in Level 2 and higher level products require the characterisation of all error sources, including specifically the input EO data (Level 1). These do not exist at per pixel level which is a big problem. In general, the knowledge of input uncertainties is poor (auxiliary data, DEM, thresholds, …). A correct error propagation requires also the correlation between uncertainties, i.e. the covariance matrix. This is also not available in general.

While the principles of calculating errors in Level 2 and higher level products is described, the implementation for a new algorithm is difficult. Proper “recipes” or best-practices are not (yet) available (H2020 project Fiduceo is working on this). Tools to easy the implementation and to work with uncertainties (e.g. in the Sentinel Toolbox SNAP) are in very early stages and need further development.

3.4.9 New Technologies

Measurement of the Particulate Scattering Phase Function and its natural variability remains a key optical parameter where there is significant lack of knowledge.

Many studies have been made in the last 15 years to measure and characterise specific inherent optical properties such as mass-specific particulate backscatter and chlorophyll-specific phytoplankton absorption and other parameters required in IOP models such as the spectral variation of CDOM and non-algae particle absorption. However, these measurements were done mainly in oceanic waters, and the impact of the natural variability and general uncertainty of these parameters on end-user products such as chlorophyll a concentration, means that measurement of such parameters remains a priority.

Radiometric data for satellite validation is very sparse, particularly for the extremely absorbing and extremely scattering water types not well covered by the AERONET-OC network.

In many extremely scattering and absorbing waters the retrieval of phytoplankton absorption or chlorophyll a concentration remains a severe challenge and it is generally difficult to satisfy user needs for more detailed phytoplankton information by remote sensing alone. Information on phytoplankton species distribution or functional type is generally not available. In extreme waters, it will always remain a very big challenge to detect small signal variations by different species when TSM and CDOM are at extreme high values.

3.5 Research and Development Priorities

From the previous chapter it is evident that further development is required at spaceborne and in-situ instrument level, protocols, algorithms and validation. The participants discussed actions needed to improve the products as well as outreach to users, and priorities.

Four main lines of actions were identified:

1. **Better characterisation of water and atmosphere specific optical properties (quantity, quality, geographical coverage), including the vertical dimension, with harmonised protocols and new instruments;**

2. **Improving atmospheric correction and in–water retrieval algorithms by using the improved SIOP data of atmosphere and water and by exploiting the new spectral features of Sentinel 3 and Sentinel 2 sensors.**

3. **Optical water type classification, to be used for algorithm selection as well as water type identification**

4. **Development of agreed, comparable measures of uncertainties and supporting tools to derive and propagate them**

In detail the following actions should be undertaken in order to implement the above action lines. Each action has assigned to it a time frame (S = short term (0-2 years, L = long term 3 – 5 years)

3.5.1 Atmospheric Correction

Need to better understand the limits of each AC:

- Tools for easy characterization and comparison of different ACs (S)
- Develop or improve techniques to provide uncertainty estimation for each AC (S)
- Improve characterization of (S)IOPs and their impact on AC, for example (L):
    - Spectral dependency of bbp for C2SX
    - Spectral dependency of S-CDOM for C2AX
    - Improve characterization of the atmospheric and Fresnel reflection, in particular at high latitudes
    - Common database of in-situ data (radiometric) + satellite matchups

- Use this knowledge to push the limits of the algorithms (L)
- Improved Radiative Transfer modelling for atmosphere and ocean, applicable to extreme absorption and turbidity ranges (L)
- Study how (existing or potential) instrumental features can be used to improve AC (S)
    - New spectral bands
    - Directionality, polarization
    - Instrumental synergy (spectral, spatial, temporal)
    - (specific to each AC)

3.5.2 Optical Water Types

R&D priorities on theory, algorithms and methods:

- Development of methodologies for optical water type classification for (a) algorithm blending and (b) bio-geo-chemical water body characterization (S). Ensemble techniques (probabilistic solution finding of different algorithms) should also be studied (S).
- Demonstration of WFD reporting using Sentinel 2 and Sentinel 3 (S)

R&D priorities on satellite and in-situ measurements:

- Coastal, estuaries and inland water mission; upgrade of S2 with dedicated bands (e.g. 681nm, thermal bands), low SNR with a spatial resolution of 30m or better (L)

R&D priorities on data processing:

- The development and application of water type classification for algorithm selection and blending requires a flexible environment to adapt the classification to specific needs, and to run it on (large) data sets of different sensors. Ensemble techniques should be supported. Linking with reference data is necessary for algorithm calibration per water type (OWT-Themtic Exploitation Platform) (S).

General comment on organisational aspect:

- Software tools should be under an open source license in order to maximize transparency and usage.

Short term actions would address the methodological OWT work, to be demonstrated at Sentinel 2 and 3, as well as the demonstration of S2 and S3 for WFD reporting. Work to better characterise atmosphere and water should be initiated.

Long term actions should aim at preparing a dedicated inland water mission or update of Sentinel 2. Work to better characterise atmosphere and water should be fully implemented and data should be exploited.

3.5.3 Water characterisation

Beside extending the measurements to more water bodies in order to get a wider coverage with water characterisation data, most importantly is to harmonise the methods and protocols so that data become comparable. In the long term, development of new instruments and methods can lead to harmonization (L). Meanwhile, measurement campaigns should be conducted in various European and non-European water bodies (S), whereby the shortcomings can be mitigated by:

- Observing the same data processing and quality checks protocols:
    - Flags (e.g. due to poor measurement conditions)
    - Give standard deviations
- Having the same sampling strategy:
    - Optimization of sampling in time and space (e.g. to get more matchups)
    - vertical profiles: IOPs,
    - depth: ~1/2 Secchi depth, esp. stratified waters
- Making data available, open access:
    - Data policy
    - Data format
    - Complete metadata (including instrument calibration etc.)

3.5.4 Masking of Pixels

The following points need to be addressed in order to overcome existing issues and to address new challenges:

- Synergistic use of sensors in order to have more information (bands), e.g. OLCI and SLSTR for cloud screening (S)
- Geometry for cloud shadow derived from cloud classification, which need further refinement by post classification. Only few algorithms developed and not sufficient enough (S)
- Especially for inland waters, a high resolution DEM is needed in order to retrieve the shadowing effect by mountains (S)
- Combine the findings of OWT and the detection of extreme water types in order to improve cloud screening above floating vegetation or over extremely turbid waters (iterative process) (S)
- Post classification after AC for very (AC) turbid conditions (S)

A second important fields for the identification of invalid or inaccurate pixels is the warning if algorithm did not work properly. Each algorithm should provide such information. However, still invalid pixels are not correctly identified and cause artefacts or wrong results, i.e. wrong concentrations. Topics that need to be addressed this are:

- Request quality flagging from each algorithm that is provided in a toolbox (at least flagging results that fall outside of the valid range of values) (S)
- Post classification for identification of wrong pixels (S)
    - Develop methods for a proper post-classification

    - Consistency check of spatial features, e.g. homogeneity)
    - Consistency check for temporal features (realistic?)
- Develop methods to integrate the uncertainty information of the products (L) into the final products (matter of validation, investigation which accuracy needs a warning, which an exclusion from the current data set.

General comment on organisational aspect: A protocol is required that applies to algorithms and describes how information about their validity ranges, conditions under which they work/don't work, how uncertainty is derived, should be provided.

3.5.5 Chlorophyll–a and CDOM products

The quality of Chlorophyll and CDOM retrieval needs to be improved. More in-situ data in extreme Case 2 waters is required to validate the algorithms. Different algae species composition needs to be taken into account in the inversion algorithms. This can be achieved e.g. by pre-processing with an OWT to guide to the most likely phytoplankton model.

3.5.6 Carbon related products

The theory for POC-algorithms needs improvements. In Case-1 waters the source of POC is phytoplankton and organic detritus, for coastal and inland waters it is additionally related to organics bound to suspended matter. For coastal waters an algorithm is needed which uses absorption and scattering simultaneously (L).
For the development of this algorithm for coastal and inland waters the correlation between optical properties and POC has to be investigated (L).

As the DOC-retrieval relies on the CDOM-determination, there is no extra effort necessary – except validation. It has to be mentioned that there are waterbodies where there is no correlation between CDOM and DOC and such algorithms do not work. This requires match-up with in-situ data of POC and DOC in coastal areas. DOC-CDOM matchups are needed for lakes to validate if the CDOM can be used for DOC estimation or not. POC plays a little role in lakes where more than 90% of carbon is DOC.

3.5.7 Non–concentration products

From precursor work and requirement studies, a certain set of products can be defined for which algorithm should be developed:

- Indicators (L4 products)

    - Combining EO and e.g. biological or physical chemical data
    - Trophic state classification
    - Merging of data sources
- Statistical analysis of time series to further explore the potential applications
    - Phenology
    - Phenology in support of water body typology
    - Trend
    - Identification of exceptional events
- Pattern recognition
    - HABs occurrence, position and extent
    - Feature identification and frequency of occurrence
- Development of monitoring concept for in situ and EO integration
    - Planning of in situ campaigns
    - Sampling strategies (stratified sampling schemes)

3.5.8 Uncertainties

The developments in other disciplines (e.g. SST) should be analysed and transferred to ocean colour (S).
Proper tools for describing the uncertainty budget (with quantification) should be developed, and combined with tools to include this in error propagation. (S)
Because a full model of uncertainties will be impossible in general, a methodology to estimate the uncertainty of products by Monte-Carlo methods should be developed (L).

3.5.9 New Technologies

Improvements on Sentinel–2 class instruments?

Due to their dynamical nature, the case2x waters require frequent, high-quality, and consistent observations. Recognizing that the 10-30m resolution is sufficient for capturing the spatial variability of these water types in most ecosystems, following improvements are highly recommended for the future Sentinel-2 class (E & F) missions:

- SNR: Although designed primarily for land science applications, Sentinel-2 (and Landsat-8) has shown promise for applications in case2x waters. However, low SNR (across the VNIR+SWIR) over these relatively dark waters generally limit utility of water quality products. High-noise in the SWIR bands, in particular, introduces noise in the retrieval of products through the atmospheric correction process.
- Spectral coverage: While a hyperspectral instrument is desired, priority can be given to the addition of bands centered at ~410nm (to improve CDOM retrieval), 620nm (to quantify cyanobacteria blooms), 810 nm (dip in absorption of water molecules allows to

estimate scattering particles – phytoplankton (Chl-a) or SPIM, depending on the dominance) are desired. Narrowing the existing bands can also help capture finer spectral features in Level-2 products, which eventually improves the retrievals of water quality parameters.

- Pre-launch characterization: Assuming a constellation of Sentinel-2 class missions (e.g., Landsat + Sentinel-2), a consistent characterization of the instruments at low-radiance radiometry is recommended. Characterization of non-linearity at low radiance levels and of the spectral responses for all the detectors is highly recommended.
- Onboard calibration procedures: The use of darker solar diffuser panels (e.g., ~10%) for characterization of low-radiance levels is recommended.
- Glint avoidance: Sea-surface glint and high-backscattering haze continue to hamper high-quality products (e.g., coral reef distribution) derived in low-latitude regions. Therefore, westward/northward tilting of the instrument is recommended.

In–situ

Development of the new generation of in situ instruments including improved hyperspectral radiometers covering at least the UV/VIS/NIR range (350-900nm) for satellite validation, automated sunphotometers and sky cameras, automated flow cytometers and/or spectrofluorimeters for phytoplankton species, volume scattering function meters, and backscattering and absorption meters adapted (e.g. with short pathlength) for extremely scattering and absorbing waters.

Improved integration of autonomous instruments into standardized networks and coverage of extremely absorbing and scattering waters by such networks.

Session 4: Satellite Measures Assessing Phytoplankton Diversity on Global and Regional Scale

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This report provides a scientific roadmap for future directions for research and development of satellite measures assessing phytoplankton diversity on global and regional scale that emerged during the presentations (oral and poster) during the **"Phytoplankton Diversity at Global and Regional Scale"** Session and the corresponding Discussion Session at the CLEO workshop at ESRIN on 6-8 September, 2016. This session and its discussions were organized within the context of activities of the ESA Scientific Exploitation of Operational Missions (SEOM) SY-4Sci Synergy R & D Study 4: Phytoplankton Functional Types (SynSenPFT, see CLEO presentation by Astrid Bracher). This report was written by a group scientist participating in this session. The discussion session started with the following seed questions:

1. Do existing satellite phytoplankton diversity products meet the requirements of the user community?
2. What can be done to serve better the needs of the user community
3. How should the information obtained from different sensors and the different satellite products be merged so it meets the requirements needed by users?
4. What additional products (from in-situ and modelling) should be added to the product streams to increase the usefulness of satellite PFT products?

4.1 User needs for measures of phytoplankton diversity from space

Marine phytoplankton play an important role in the global carbon cycle via oxygenic photosynthesis and the carbon biological pump and contribute to ~50% of the global primary production. Over the past 30 years, ocean colour remote sensing has revolutionised our understanding of marine ecosystems and biogeochemical processes by providing continuous global estimates of total chlorophyll *a* concentration (chl-a), used as a proxy for phytoplankton biomass. However, chl-a does not provide a full description of the ecosystem alone. Phytoplankton have different morphological and physiological characteristics and different biogeochemical and ecological functions. Differences in phytoplankton community structure are thus important to many fundamental biogeochemical processes, including: nutrient uptake and cycling; transfer of energy through the marine food web, deep-ocean carbon export and even the emission of chemical compounds to the atmosphere (which then e.g. form cloud nuclei or are involved in ozone destruction). Phytoplankton community composition has important consequences for fisheries and specific species can directly impact human health (e.g. Harmful Algal Blooms = HABs).

The ability to observe the spatial-temporal distribution (phenology) and variability of phytoplankton groups is a scientific priority for understanding marine food web, and ultimately predicting the ocean's role in regulating climate and responding to climate change on various time scales. Thus, to identify the drivers of phytoplankton composition on global and regional scales is required to assess climate and ecosystem interactions, but also to increase our understanding of the role of the ocean's biodiversity. These high coverage data sets on phytoplankton diversity are especially urgent for many socio-economic applications (e.g. fisheries, aquaculture, and coastal management). Coasts are especially vulnerable to major human threats caused by HABs, eutrophication, and other measures deteriorating water quality.

To better reflect the impacts of different phytoplankton for ocean biogeochemical cycles, Earth System and climate models, including those used in the IPCC assessments, have increasingly included a larger amount of biological complexity in their ocean component. To simplify the representation of the vast diversity of phytoplankton and zooplankton, they are typically grouped according to their biogeochemical functions (plankton functional types). Models now commonly include 3-10 plankton functional types, with several models representing up to 100 or more plankton types defined according to biogeochemical function and/or other physiological characteristics. Since in-situ data is scarce and many vast ocean regions are too remote to be routinely monitored, models are strongly reliant on estimates of phytoplankton functional types (PFTs) from satellite observations in order to reduce the large uncertainty in their projections of future changes in net primary production, or carbon export. Information on phytoplankton community composition (including PFT distributions) from ocean colour satellites is therefore highly desirable for model validation or for assimilation into these models.

In turn, a better understanding of the phytoplankton community composition on broad temporal and spatial scales accomplished by in-situ observations, numerical modelling and remote sensing will improve in water radiative transfer modelling and by that improve retrievals of other variables from ocean colour (since absorption and (back)scattering properties also change significantly among different types of phytoplankton).

Recommendation: Satellite data on phytoplankton diversity obtained from ocean colour is urgently needed (instead of just chl-a) to improve near-real time and forecasting models for assessing and predicting climate change and marine services facilitating the above mentioned management needs. Users request ocean colour (OC) data on phytoplankton diversity (see session "Ocean colour applications for climate studies") as essential climate variable (ECV) and efforts have to be taken to incorporate it into the ocean colour climate change initiative (OC-CCI).

4.2 State of the Art in Estimating Phytoplankton Diversity from Space

The CLEO overview talk by Stephanie Dutkiewicz on "Modelling diverse phytoplankton communities" it was pointed out that diversity of phytoplankton is large and can be characterized by multiple dimensions (e.g. size, biogeochemical function, nutrient uptake, accessory pigments, morphology, thermal niche, predation protection or avoidance, symbiosis, etc.). Even within a species there are often a large range of ecotypes. Scientists tend to group large number of species together depending on the purposes of their research. For instance those with climate level numerical models will contemplate several PFTs based on their biogeochemical function (e.g. diatoms with strong effect on the silica cycle, nitrogen fixers as important players in the nitrogen cycle). Here, we refer (based on satellite outputs) to any clustering of species (and ecotypes) as "Phytoplankton Groups" (PG). PG characterised by a certain taxonomic group we name phytoplankton types (PT), and by a size range we name phytoplankton size classes (PSC).

The CLEO presentation by Julia Uitz in the session "**Phytoplankton Diversity at Global and Regional Scale**" gave an in depth overview on "Retrieving phytoplankton diversity from ocean colour observations" (see also recent summary in IOCCG 2014). Ocean colour algorithms to assess phytoplankton diversity make use of information originating from phytoplankton abundance, cell size, bio-optical properties to differentiate PT and PSC Abundance based approaches use satellite chl-a as input to derive PSC or PG based on empirical relationships of in-situ marker pigments to chl-a (determined using high precision liquid chromatography, HPLC)). Another class of algorithms relies on spectral features caused by the variation in phytoplankton composition either observed in changes in reflectance or derived absorption and/or backscattering spectra. A third approach further incorporates various environmental parameters to predict PT based on their ecological characteristics. Products obtained from these algorithms are typically dominance, presence or absence of a certain PG, or fraction or chl-a of the three size classes. Currently, only products by OC-PFT (Hirata et al. 2011, CLEO presentation by Annalisa Di Cicco) and PhytoDOAS (Bracher et al. 2009, Sadeghi et al. 2012, CLEO presentation by Julia Oelker) enable the simultaneous determination of chl-a of several PTs. PhytoDOAS retrieves the imprints of specific phytoplankton groups' characteristic absorption among all other atmospheric and oceanic absorbers from top of atmosphere data of the hyperspectral satellite sensor SCIAMACHY (Scanning Imaging Absorption Spectrometers for Atmospheric Chartography). All other PG algorithms have been applied to multispectral satellite data (e.g., Sea-viewing Wide Field-of-view Sensor (SeaWiFS), Medium Resolution Imaging Spectrometer (MERIS) and Moderate Resolution Imaging Spectrometer (MODIS)) using water leaving reflectance data.

Several of these algorithms have been used in wider applications; mostly for evaluation of biogeochemical/ecosystem models, but also beyond (e.g. inferring oceanic emissions of volatile organic compounds, harmful algal blooms). Quite a few of these PG algorithms have been inter-compared globally: Firstly they were inter-compared using in-situ PSC data (derived from HPLC) in terms of dominance (Brewin et al. 2011). Secondly, the spatial variability of diatom and microphytoplankton phenology was compared (Kostadinov et al., in revision) under the 2nd Satellite PFT Algorithm International Project (project website: http://pft.ees.hokudai.ac.jp/satellite/index.shtml). This project accommodates four working groups (WG): (1) User Guide WG, (2) *In–situ* Data WG, (3) Inter-comparison WG, and (4) validation. A user guide on these algorithms has been written (Mouw et al. submitted), and a global in-situ dataset of HPLC and optical properties is being developed to further evaluate the algorithms. This initiative organized at the International Ocean Colour Symposium (IOCS) 2013, the IOCS 2015 breakout sessions and in 2014 a specific expert International Ocean Colour Coordination Group (IOCCG) workshop focusing on PFT algorithms, validation and related user needs. As a summary of these meetings recommendation for actions and future planning were given (see reports given at IOCS and IOCCG websites).

In the last years, radiative transfer models (RTM) and ocean reflectance models (ORM) have been used to develop and assess the sensitivity of analytical retrievals for PTs or to find suitable spectral characteristics necessary for ocean colour sensors to retrieve PGs. ORM studies showed that with current multispectral sensors only presence or absence of certain PT can be retrieved. Recent ORM simulations (see CLEO poster by Aleksandra Wolanin) showed that only by adding to a sensor like Ocean Land Colour Imager (OLCI on Sentinel-3, S-3) four more bands (381, 473, 532, 594 nm) or using hyperspectral data at moderate spectral resolution (5 nm) will enable to retrieve chl-a of several PT in case-1 waters. However in complex waters, as shown by RTM, it seems only presence or absence of PT can be retrieved or not even that since it is masked in extreme complex waters (see CLEO session "**Turbid Waters and Highly Absorbing Waters**") by the strong absorption and/or scattering of other water constituents (coloured dissolved organic matter (CDOM), total suspended matter (TSM)). Recent methods have been developed to retrieve PT or PSC from hyperspectral algal or particulate absorption coefficients, and validated using in-situ measurements. As absorption coefficients can be derived from satellite measurements using inverse bio-optical models, this opens the way to an application of these methods to ocean colour.

To date, the majority of existing PG satellite retrieval approaches have utilized HPLC pigment relationships to derive in-situ data on PT or PSC (e.g., see CLEO presentation by Florinda Artuso), respectively. Large in-situ PT and PSC data sets have been compiled for developing and validating algorithms using publicly available pigment data (MAREDAT), complemented by recent submissions to SeaBASS, BATS. LTer, AESOP, PANGAEA. HPLC-phytoplankton pigment data are the largest and have the highest spatial coverage with standardised quality control protocols. However, size fractionated data of chl-a serve as a more direct validation data set for assessing satellite retrievals on PSC. In addition, phytoplankton group specific IOPs (absorption and backscattering) measured in the field or in cultures have been used as algorithm inputs. The large regional continuous plankton counter data sets have been used for constructing and evaluating ecological algorithms focusing on larger phytoplankton. Inline (coupled) flow-cytometry and microscopy techniques have developed and enable a more precise classification of the phytoplankton groupings than by HPLC marker pigments. Hyperspectral IOP measurements can help in validating by increasing the number of match-ups and assessing PG variability within a satellite pixel and quantifying the uncertainties in the two-step satellite methods.

Numerical modellers are one of the “users” targeted for ocean-colour PG products. Starting over two decades ago, biogeochemical models began incorporating multiple phytoplankton groups mainly to incorporate their biogeochemical relevance. For instance, as a first step models incorporate a “diatom” group given their importance in the silica cycle, but also given the expectation that they were more important to carbon export than other phytoplankton. As models developed more appropriate nitrogen biogeochemistry, many additionally included a “diazotroph” class. Given the different biogeochemical importance of these groups of phytoplankton, the modelling community refers to these modelled groups as PFTs. These models therefore correspond most easily to OC PT products that target biogeochemical function. One disadvantage of this approach is choosing the parameters governing growth and loss of PFTs in the model. For instance, laboratory studies have found maximum growth rates of different diatom species vary from one to four per day which makes it difficult for a modeller to choose a value for a diatom PFT. Though less common, models can group phytoplankton in terms of size which compares more easily with OC-PSC algorithms. It is also an advantage that such an approach can use empirical allometric relationships of key growth parameters (e.g., maximum growth rates).

Since 2009, marine ecosystem modellers collaborate in the MARine Ecosystem Model Inter-comparison Project (MAREMIP), specifically targeted at fostering the development of models based on PFTs in order to progress towards the resolution of important scientific questions related to biogeochemistry and ecology, and to promote the interactions between modellers and observationalists and the development of targeted observations. Complementary to the CMIP5 and CMIP6 efforts, MAREMIP thus specifically targets the inter-comparison of the representation of present and future marine biology in global ocean models. MAREMIP, as well as many single model studies conducted by marine ecosystem modellers worldwide have used satellite-derived PT products for evaluating model performance, and the community is increasingly comparing these multiple model PFT products to in-situ data products compiled for each PFT within e.g. the MAREDAT initiative.

4.3 Gap Analysis and Research and Development Priorities

Currently satellite products on phytoplankton composition are not in a format to be used among a wide user community. In the following we detail the gaps to meet the scientific questions and user needs and give recommendations for actions which define the research and development priorities.

Gap 1: Mismatch between satellite products and user needs

At present, there is a clear mismatch between the definition of PGs detected by algorithm developers and the grouping required by the user community. There are also substantial differences in the PG definitions among users. While for most biogeochemical models and RTM a quantitative assessment (e.g. given as concentration of chlorophyll or carbon) of PT is needed, end users for managements in coastal environments need PG products as indicators (e.g. of water quality, HABs, eutrophication, fisheries). Although the initiative of the 2nd Satellite PFT Algorithm International Project has led to much stronger links between algorithm developers at global scale and action has been taken towards preparing a user guide on some algorithms (e.g. IOCCG 2014, Mouw et al. submitted), these activities have been limited by low levels of funding. Furthermore, the user community requests a user guide on the differences between PG algorithms, and their use in a variety of applications, with advantages and disadvantages of different algorithms discussed in detail, and uncertainty estimates associated with each of the algorithms reported. In order to better constrain present and future estimates of marine ecosystem functioning and ocean biogeochemistry in the next IPCC assessment, much improvement is needed in terms of the representation of PFTs in the current generation of models. Furthermore, as the community is moving towards models of increased complexity, information on phytoplankton community composition from space including all PGs, or other indices of biodiversity (e.g. by PSC) provide valuable resources for the next generation model users. There is thus a need for on-going product development along with effective communication between remote-sensing scientists, observationalists and modellers to ensure that future developments are consistent and comparable, and thus that climate predictions are as robust as possible.

Recommendation to improve match between satellite products and user needs: A mechanistic framework to get a consensus on specific PGs needs to be put in place. This will assure that users are aware of the actual specific groups in the different satellite products and how they compare to the groups they have in their specific application (e.g. models). Such a framework requires an international effort (and funding) and needs to involve experts from in-situ (HPLC, microscopy, flow-cytometry, genetics, biooptics), algorithm developers and representatives of the user communities (modelling, marine services). Certain medium-term actions should take place:

- Regular **workshops to improve communications** between users (biogeochemical-, ecosystem-, RT- & OC modellers, taxonomists, ecologists, fisheries, HAB, water quality) and producers to achieve common understanding on a consistent comprehensive definition of the “groups” in PG and PSC algorithms, but also their metrics (% versus chl-a (or carbon) conc. vs. dominance), potentially leading to possible joint future proposals.
- **Website** informing on PG algorithms activities (user guide, algorithm inter-comparison and validation protocols, forum, …).
- A **“living” user guide** (continuously update) on available PG algorithms and satellite products including definition, uncertainty, strengths and limitations.

Gap 2: Lacking traceability of uncertainties in PG algorithms

The quantitative assessment of uncertainty in PG satellite products is still insufficient. This is due to limitations in appropriate in-situ data (see Gap 2a), the above mentioned mismatch definition (see Gap 1), the limited theoretical background and error by the spatial and temporal upscaling of specific PG signatures of diverse communities (see Gap 2b).

a) due to missing in–situ capabilities

Currently, the use of available in-situ data challenges the quantitative assessment of uncertainty in PG satellite products*:* Firstly, to date the majority of the existing PT and PSC satellite retrieval approaches have utilized HPLC pigment relationships with taxonomic groups or size classes. However, inputs to these data sets are accessory pigment concentrations, which only to a certain degree are congruent with taxonomy or phytoplankton size. Size can vary a lot within functional or taxonomic groupings, e.g. diatoms can range from 3 µm to 500 µm. Similarly, grouping by accessory pigments can be problematic as there is substantial variability in pigment concentration as a function of the environmental conditions independent of PG. Moreover some PGs, e.g. coccolithophores, can't be easily inferred from HPLC pigments. In consideration of the expanding satellite sensor capabilities, there is a need to begin to define coordinated efforts to compile and generate comprehensive in-situ datasets (not just HPLC). There is also a need to provide best practises to merge the different types of datasets (e.g. HPLC, microscopy, flow cytometer) into a coordinated product that simultaneously enveloped different ways of grouping phytoplankton species.

Recommendation for curation and acquisition of in–situ data sets and development of new in–situ technologies to enable assessment of PG retrievals uncertainty and their further development

1) Within international cooperation of space agencies the **curation of existing measurements of in–situ** PT and PSC abundance (HPLC, microscopy, flow-cytometry, genomics, …), and corresponding optical (inherent optical properties (IOPs), apparent optical properties (AOPs)) data needs to be secured, specifically:

- A coordinated **selection of specific comprehensive datasets** that include coincident IOPs, AOPs, and phytoplankton composition should serve as a resource for PG algorithm development, refinement and validation, and improve the ability to inter-compare validation metrics.
- **Standardized data quality and format among different data bases** (e.g., SEABASS, MERMAID, PANGAEA, AESOP, …) should be assured to enable easy compilation and expansion.
- **Methods to convert from in–situ** (e.g. pigment) data **to PT and PSC biomass** (carbon, chl-a) should be assessed and **protocols for merging different datasets** (e.g. HPLC, microscopy,…) should be formulated.
- Utilize (and **sustain) existing time series sites** (that cover a range of oceanic regimes, including coastal ocean) rich in phytoplankton composition information.
- Curate existing relevant (**hyperspectral and/or PG related) IOP data from laboratory studies**.

2) There is a need to support directed **programmes for sustained in–situ data acquisition,** to secure assessment of accuracy of PG and related (e.g. atmospheric correction, CDOM, TSM) satellite products. This includes

- advancing the knowledge of phytoplankton composition by **protocol standardization** for in-situ data collection and processing by internationally run round-robins and calibrations with at first focusing on HPLC-pigment (as done by a NASA WG updating the SEAHARRE report), second on the assessment of methodological errors associated with different approaches measuring phytoplankton absorption (as done by a current NASA WG) and then on other PG- and optical in-situ techniques (flow-cytometry, microscopy, particle scattering, radiometry),

- fostering **validation of new launched ocean colour sensors (particularly now OLCI/Sentinel–3) across all AOPs and IOPs to PG** associated measurements by sustained funding,
- adding other **in–situ techniques assessing phytoplankton composition** to existing time series sites,
- and **identifying target locations** for future field sampling (informed by existing products' uncertainty assessments and supported by modelling)

3) For increasing the spatial and vertical coverage of measurements **new technologies for in–line and autonomous measurements** should be supported via the use of **robotic platforms** (e.g., profiling floats, autonomous surface water vehicles) and the **development of new miniature sensors** that can be deployed on these platforms to provide accurate measurement of phytoplankton community and carbon (e.g. miniature imaging flow cytometers, sensors for metagenomics hyperspectral IOPs and AOPs) to ensure appropriate evaluation of satellite PG products performance on their spatial and temporal resolution.

b) due to an incomplete theoretical background

The theoretical background to connect optical signatures to diversity of phytoplankton communities across different environments is still insufficient, especially for complex waters. This limits not only the development of PG retrievals based on inversions, but also limits the assessment of uncertainties in the algorithms. At the cellular level, a detailed understanding of how pigment packaging and pigment composition that combined govern the shape and magnitude of chlorophyll specific absorption (especially in the blue-green regions of the spectrum, which is commonly used in PG algorithms) still requires further understanding. Both, reconstruction and decomposition, methods are often applied separately to bio-optical datasets to explore the link between pigments and phytoplankton absorption. Reconstruction approaches conventionally apply a single pigment-specific absorption coefficient to a particular pigment or pigment type (e.g. photosynthetic and photoprotective carotenoids), often obtained from measurements of extracted pigments in solvent. Only a handful of studies have examined the absorptive properties of pigment-protein complexes, yet differences in the spectral shape once pigments are embedded in proteins can be significant. Improved models on phytoplankton photoacclimation combined with new approaches in determining particle size should assist in improving our understanding of how pigment packaging influences the spectral signature of natural phytoplankton assemblages. Efforts inverting hyperspectral reflectance and absorption spectra to obtain PTs have shown quite limited success, leading only to identifications of appearance of certain PT, size class identification or to quantification of some accessory pigments in addition to chl-a. PG specific absorption properties are available but large spectral variability is related to algal culturing and variations in pigment composition and pigment packaging due to physiological responses of PG. In contrast, due to high measuring uncertainties spectral scattering properties (including back-scattering and volume scattering function) are even far less known. Thus, PG related specific IOPs are not adequately represented in RTMs. This further limits tracing back the uncertainty in algorithms.

A minority of global numerical models resolve the bio-optical properties of different PG. Several studies have demonstrated that adding spectrally-resolved optics to biogeochemical models improves model skill as well as comparability to observed optical properties. These advancements may provide a way forward for connecting more specifically with a larger range of OC-PG products.

Recommendation for improving theoretical background to enable assessment of PG retrievals uncertainty and their further development

1) The **development of a framework for clear traceability of uncertainties in PG satellite products** needs to be supported by the **specific assessment of mismatch definition, in–situ error, retrieval error, or errors due to the spatial and temporal upscaling of specific PG signatures in diverse communities**. This requires the steps mentioned in the previous paragraph on matching the user needs (recommendations given at Gap 1) and in-situ data (recommendations given at Gap 2a), but also steps linked to improving algorithm (see later Gap3 and its recommendations) and theoretical background development:
- **Inverse modelling to reach from AOPs via IOPs to PG quantitative information** via RTM needs to be optimized by improving the optics via implementing knowledge gained by measurements on spectral specific IOPs (in particular scattering properties) on natural and cultured PT and PSC samples.

2) The **mechanistic understanding to integrate the OC–PG information to user needs** has to be improved by a **better utilization of expertise** of e.g., taxonomist, molecular ecologist for interpretation of diversity and it links to PG optics. The **usage of global numerical models which resolve the bio–optical properties** of different PG will provide a way forward for connecting more specifically a larger range of OC-PG products. Models could group their model phytoplankton-analogues according to more dimensions of diversity (e.g., accessory

pigments, scattering characteristics etc.) that link closer to the OC-PG definitions than the more classical PFT designations. Models that include spectrally-resolved optics and bio-optical properties of phytoplankton could also prove to be a powerful tool for exploring the inter-dependency and regionally varying skill of different OC-PG approaches.

Gap 3: Missing capabilities of current satellite measurements

Although certain PTs have specific marker pigments, the differences among PTs in their spectral absorption are small, since many PTs contain many of the same pigments or pigments of similar absorptive properties. Given the limited number of wavebands and the broad band resolution, multi-spectral sensors can provide only limited information on the variability in phytoplankton spectral absorption caused by shifts in community structure. This restricts all multispectral satellite phytoplankton composition products based on spectral principles to either indicating dominance, presence or absence of PGs or identifying major size class fractions within the total phytoplankton community and to a high level of uncertainty.

The capability to retrieve quantitatively major PT based on their optical signature has been clearly shown with the PhytoDOAS method in the open ocean using hyperspectral satellite data from the atmospheric sensor SCIAMACHY (on Environmental Satellite (ENVISAT). However, the exploitation of hyperspectral satellite data for ocean colour applications has been so far very limited because hyperspectral sensors like SCIAMACHY (spectral resolution 0.26 to 0.44 nm) do not provide operationally water leaving radiance products and have very large foot-prints (30 km by 60 km per pixel) and low global coverage (six days). This limits to properly assess the retrieval's accuracy with in-situ point measurements, but also the application of such PT satellite data sets. The difficulty of working with SCIAMACHY data is that one has to handle strong atmospheric absorbers and heterogeneity of big pixels; hence, the PhytoDOAS algorithm was designed to retrieve diatoms, coccolithophores and cyanobacteria directly from top of atmosphere radiances, by separating their high frequency absorptions from each other and relevant atmospheric absorbers, while accounting for broad band effects by using a low order polynomial. The hyperspectral ocean colour sensor Hyperspectral Imager for the Coastal Ocean (HICO) provided low global and spatial coverage data, but very good spatial resolution. However, so far developed atmospheric correction for HICO (see current implementation in SeaDAS) failed to be able to exploit the full spectrum which would have enabled to retrieve single or multiple PGs. Eventually, not much more than standard ocean colour products as for multispectral data were derived. In general it is a big challenge to provide spectrally consistent high quality atmospheric correction for PG retrievals: it require very low uncertainty of water leaving radiances to separate the PG signatures from first order dominating absorption and scattering by the bulk parameters (total biomass, CDOM, TSM, water).

SCIAMACHY data acquisition has ended with the lost contact to the ENVISAT satellite (Apr 2012). First results from adapting the PhytoDOAS method to the Ozone Monitoring Instrument (OMI) sensor (measuring since 2004 from AURA) are very promising (see CLEO presentation by Julia Oelker) to enable the extension of the spectrally derived PT data on diatom, cyanobacteria and coccolithophore chl-a into the future with much improved global coverage (daily) and small foot print (13 km x 24 km). OMI is also the precursor instrument to the in later 2016 Sentinel-5-Precursor (S-5-P) TROPOspheric Monitoring Instrument (TropOMI) and in the 2020s launched Ultra-violet/Visible/Near-Infrared Instruments (UVNs) on S-4 and S-5 (all with pixel size 3.5 km x 7 km). S-4 is a geostationary satellite which will enable much higher temporal resolution of PG data for the disk seen by the sensor. However, still also those sensors spatial capabilities is limited and higher spatially resolved ocean colour sensors with improved spectral capabilities are needed: The new sensor OLCI on Sentinel-3 already provides two more bands for ocean colour and it is expected that the number will even further increase for future (multispectral) ocean colour sensors. In addition, very soon hyperspectral missions like Pre-Aerosol, Clouds, and ocean Ecosystem (PACE, global, high coverage, 1 km pixels, launched 2022?) and Environmental Mapping and Analysis Program mission (EnMAP, regional, low coverage, 30 m pixels, launched 2019?) are planned to start operating. However, hyperspectral instruments like EnMAP or PACE with 5 nm resolution (which is probably sufficient for ocean colour applications) are still very different from atmospheric instruments like SCIAMACHY, which have spectral resolution around 0.5 nm. Hence, the new algorithms will have to be developed (or adapted) to retrieve PGs from these new instruments.

The development of long time series of PG satellite products has just started. Such data sets are necessary to secure meeting user needs. Merging has been successfully done for several operational OC products to ensure long-term data (e.g. see GlobColour-(www.hermes.acri.fr) and OC-CCI (www.oceancolour.org) products). Several multispectral PG algorithms have been applied to more than one sensors and also to merged sensors remote sensing reflectance or chl-a products (see Mouw et al. submitted). In order to obtain high spatially and temporally resolved PT chl-a data by also using their spectral imprints into high spectrally resolved satellite data, the ESA project SynSenPFT developed a method by synergistically using PT information from SCIAMACHY-PhytoDOAS and OC-CCI-OCPFT retrievals to obtain a global PT data set from 2002 to 2012 at 4 km resolution (see CLEO presentation by Astrid Bracher).

Recommendation to obtain long–term data on phytoplankton composition at adequate temporal and spatial resolution based on the following mid-term actions incorporated into the OC-CCI tasks:

1) Foster the **exploitation of hyperspectral data**:
- In preparation for the exploitation of future hyperspectral ocean colour sensor (PACE, EnMAP or Hyperspectral Infrared Imager (HyspIRI) and hopefully more) missions, much more effort needs to be put into the **development of atmospheric correction for hyperspectral satellite data**: Methods should be developed over open ocean and complex waters and with the help of RTM and considering multispectral correction methods (e.g. POLYMER) current hyperspectral satellite data sets, such as SCIAMACHY, HICO, OMI, (and from 2017 also TROPOMI), should be explored.
- Set-up a **long time series of hyperspectral PT data**: Develop or extend hyperspectral and quantitative spectral PT algorithms to former (e.g., SCIAMACHY and HICO), current (e.g. OMI) and soon upcoming (TropOMI) to secure a global PT time series based on hyperspectral data from 2002 into the future.
- Explore the **potential of spectral PG quantitative satellite retrievals for future satellite sensors** based on further assessment via RTM, hyperspectral satellite and in-situ data: test algorithms for retrieving as many as possible PGs requested by user needs from hyper- (e.g., **PACE, EnMAP, HYSPIRI**) and multispectral data sets with e.g. 10 or more bands. An option to test such retrievals could be applied to OLCI data set with covering even more bands which is, in principal, possible to change in future Sentinel-3 OLCI instruments settings. This could be studied via an operation change request with respect to various spectral band settings for a short period of time during **Sentinel–3B** commissioning phase.

2) Set-up a **framework on international level for integrating different sensors** (hyper-/multispectral, global coverage/high spatial and/or temporal resolution) PG information to meet user requirements across different scales **with special focus to regional applications**:
- Start with a workshop to define and execute round-robins on regional (thematic) assessment of algorithms (validation, uncertainties) with defined protocol.
- Develop a best practice to use different kind of PG data to obtain synergistic PG information.
- Use merged hyperspectral PG data with low spatial resolution (from 2002 until today incl. Sentinels) for building up **high spatially resolved PG long–term global data** by synergistic use with multispectral derived PG products (incl. Sentinel-3). Optimize retrievals on trigonal scale based on other environmental and ecological information (e.g. from remote sensing, climatology, …) such as sea surface temperature (SST),

available light (PAR), wind speed, mixed layer depth (MLD), nutrients fluorescence, and optically active water constituents (CDOM, TSM) and better links to biogeography.

Based on the outcome of these two medium-term actions **new missions should be prepared to launch satellite sensors with hyperspectral (5 nm resolution) and advanced multispectral (10+x bands in the visible)** which will ensure the prolongation of PT time series at high spatial and temporal coverage and resolution (see also Gap 4).

Gap 4: Lack of regional capability

So far, PG algorithms work globally or regionally (some of them have been validated on restricted regions), but nearly all of them are limited to open ocean conditions (so-called case-1 waters). However, PG products are also needed for coastal areas and inland waters where water quality and HABs issues are most urgent. In these waters (case-2 waters) no correlation between the amount of optical constituents exist and generally OC retrievals are challenging: Phytoplankton pigment absorption can be masked by CDOM in the blue and up to yellow-green wavelengths which in the most extreme (high CDOM, low scattering) cases leads to masking of optically active signatures in the whole visible spectrum with in general very low water reflectance compared to atmospheric reflectance values. By contrast the main problems in case-2 scattering waters are the masking of pigment absorption by non-algal (organic and mineral) particle absorption and significant near infrared water reflectance (see section Case-2 Extreme). The success of obtaining successful PG data in these regions is hampered by limited spatial and spectral resolution but probably also by the signal-to-noise capabilities of sensors. In these waters it is already a challenge to obtain successfully ocean colour standard products starting with an accurate atmospheric correction. Current spatial resolution of ocean colour sensors inhibits observations of smaller assemblages of phytoplankton communities. Exploitation of additional data (light, temperature, nutrients,) to constrain retrievals and optical modelling for specific regions has been limited and specific in-situ data are missing to adapt and validate regional retrievals.

Recommendations to lower uncertainties of PG algorithms for specific regions and especially in complex waters

1) Invest in the **development of synergistic PG products from multi– and hyperspectral sensors with high global coverage** (e.g., OLCI, PACE, OMI, TropOMI, ….) and **with high spatial resolution** which have been, are or will be, operating (e.g., Landsat, HICO, MultiSpectral Instrument on S-2, EnMAP, HyspIRI) also invest in good atmospheric correction for those data sets (see Gap 3).

2) **Optimize** the regional PG outputs (algorithms) **by constraining them based on covariation to environmental variables**. Empirical methods that rely on covariation (not on a mechanistic method) to environmental variables (temperature, light, mixed layer depth) should be explored which will help especially for HAB detection to move from OC-PG towards the specific HAB.

Cited CLEO presentations

1) Julia Uitz: Retrieving phytoplankton diversity from ocean color observations: Review of past work and possible paths for the future.
2) Stephanie Dutkiewicz: Modelling diverse phytoplankton communities.
3) Julia Oelker: Towards improved spatial resolution of hyper-spectral PFT products.
4) Astrid Bracher: Synergistic exploitation of hyper- and multispectral Sentinel-measurements to determine Phytoplankton Functional Types at best spatial and temporal resolution (SynSenPFT).
5) Annalisa di Cicco: Specialized Empirical Algorithms for the Identification of Phytoplankton Functional Types and Size Classes in the Mediterranean Sea.
6) Aleksandra Wolanin: Towards Improving Phytoplankton Functional Types (PFTs) and Standard Chlorophyll-a Retrievals.
7) Florinda Artuso: Measurements of pigment composition in the Mediterranean Sea, a contribution to the Sentinel-3 Cal/Val activities.

Other References

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Session 5: Pools of Carbon in the Ocean

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5.1 Introduction

This report provides a scientific roadmap for the use of, and priorities for, ocean-colour products in carbon-cycle research that emerged from the presentations (oral and poster) during Session 5 (Pools of Carbon in the Ocean) and during the corresponding Discussion Session at the CLEO workshop in ESRIN on 6-8 September, 2016. The carbon-related sessions and discussions were organized within the context of the activities of the Pools of Carbon in the Ocean (POCO) Project of ESA. While the project focuses on oceans, in this report also recommendations are given concerning inland waters. The discussion session began with the following seed questions:

1. Do existing ocean-colour products for particulate pools of carbon (Particulate Organic Carbon or POC, phytoplankton carbon) meet user requirements?

2. What are the known weaknesses in existing algorithms for estimating pools of particulate carbon (Particulate Organic Carbon or POC, phytoplankton carbon) from ocean-colour data? What can be done to address these weaknesses?

3. What can be learned from modelling approaches?

4. What should be our priorities for further developing improved algorithms for pools of carbon in the ocean, both dissolved and particulate?

5. What is the role of lakes in the global carbon cycle and to what extent remote sensing can be used to determine this?

5.2 Statement of Need

In the context of a changing climate, considerable effort is devoted to study of the planetary carbon cycle, through observation, analysis and modelling. It has been established beyond doubt that the ocean is a key player in Earth's carbon cycle, raising an imperative for us to quantify, in operational mode, the pools and fluxes of carbon in the ocean at the global scale with sufficient accuracy and precision to permit detection of change as the planet warms. Here we review that section of CLEO devoted to the Pools of Carbon in the Ocean. Specifically, the underlying need is to quantify the pools of particulate and dissolved organic and inorganic carbon, using remote sensing and in situ observation, and to compare the results with those arising from the numerical models that the IPCC relies on to forecast future Earth climate. Special emphasis is required to quantify the pools of organic carbon associated with living phytoplankton, because:

1. Phytoplankton are responsible for massive consumption of inorganic carbon through photosynthesis to augment the size of the particulate organic carbon (POC) pool (50 Gigatonnes per annum at the global scale); this is also the principal source for the dissolved organic carbon (DOC) pool in the ocean; and
2. The ratio of carbon to chlorophyll in phytoplankton is a key parameter in coupled ocean-ecosystem models: it is a variable property whose magnitude is as yet poorly constrained. Urgent attention is required.

Although carbon fluxes were not treated exhaustively in CLEO, primary production and export production were recurring issues in the meeting, and should be considered as cross-cutting issues.

The role of lakes in the global carbon cycle and more accurate determining of it by means of remote sensing was discussed in the meeting. IPCC recognized the role of lakes in their last report and included them as a part of global carbon cycle. IPCC used statistical estimate on the number and size of lakes (known to be inaccurate) and conservative estimates of carbon in lakes. The actual number and area of lakes has been mapped with remote sensing and remote sensing is the only mean to estimate the carbon pool in lakes that is mainly in the form of DOC. This is the field where ESA can make significant contribution.

5.3 State of the Art in Estimating Oceanic Carbon Pools by Remote Sensing

Oceans are home to a variety of particulate and dissolved, as well as organic and inorganic pools of carbon. The state of the art with respect to various pools are briefly examined below.

Particulate Organic Carbon (POC): Standard band-ratio satellite remote sensing algorithms for POC in the open ocean are generally available and globally validated. However, validation is not done as comprehensively as it is for Chl-a. The derived POC concentrations possess a similar uncertainty level as those for Chl-a. Case-1 water POC algorithms cannot be used in optically complex and "extreme" waters due to a higher proportion of POC associated with organic and minerogenic detritus that has a complex relationship with optical properties and with reflectance. Some regional algorithms exist. But no general algorithm exists, or has been validated, for Case 2 waters.

Phytoplankton Carbon (C_p): Estimations of phytoplankton carbon (C_p) are in general based on satellite-derived Chl-a or POC, but no direct estimation from RS reflectance is available yet. There are some algorithms based on inherent optical properties (mainly on the backscattering coefficient) and others are particle-size based. These approaches currently have large uncertainties and development is limited by availability of suitable *in situ* datasets. Validation of C_p has been done in only a few cases, using *in situ* data that describe only parts of the phytoplankton carbon (some size fractions, rather than the total).

Dissolved Organic Carbon (DOC):
In coastal and inland waters DOC is derived, through its coloured component CDOM. However, this is not always the case. There are waters with no correlation between DOC and CDOM. On the other hand, DOC in lakes is in correlation with pCO_2 meaning that estimating lake pCO_2 using CDOM as a proxy may be feasible. More than 90% of the carbon pool in lakes is in the form of DOC. Therefore, DOC is the most important carbon fraction to be estimated from satellites in order to determine the role of lakes in the global carbon cycle. The current estimate show, that the amount of carbon outgassed from lakes exceeds the amount of carbon transported annually from land to oceans and the amount of carbon going to lakes sediments is in the same order of magnitude with the amount of carbon transported from land to oceans.

In the open ocean, DOC is not related in any simple way to CDOM, and DOC cannot be estimated from CDOM directly. Remote sensing algorithms for CDOM and Coloured Detritus Matter (the latter combines the absorption contributions of CDOM and non-algal particles) exist for both lakes and ocean waters but require further improvements and validation for both Case 1 and Case 2 waters, especially in view of challenging problem of separating the contributions of CDOM and non-algal particles.

Particulate Inorganic Carbon (PIC): Scattering- and reflectance-based algorithms for particulate inorganic carbon (PIC) in the open ocean are established for the estimation of biogenic PIC in coccolithophore blooms, where these algae are the major source of PIC and are visible due to the strong scattering of the coccoliths. The PIC associated with SPM in coastal waters might be estimated from SPM concentrations and PIC/SPM-relationships. No direct algorithm or mechanistic approach is established for PIC in coastal waters.

Dissolved Inorganic Carbon (DIC):
RS Algorithms for dissolved inorganic carbon (DIC) are generally not well established, as DIC cannot be derived directly from optical properties although correlation of TIC with Chl-a and absorbance at 443 nm, and consequent estimation from MERIS data, has been shown in lakes. A few existing mechanistic algorithms are based on the

combination of optically-derived parameters (Chl-a), SST and SSS (in case of alkalinity).

Established algorithms for POC, CDOM and SPM have not reached a performance quality similar to that for Chl-a, thus, uncertainty estimates for the related RS products are possible. Moreover, in many optically complex waters (coastal and inland) the Chl-a algoritms need significant improvement. All available products will benefit from recent advances in satellite sensors regarding accuracy and uncertainty estimates.

5.4 User Requirements for Climate Models

The global carbon cycle is central to the functioning of the climate system and the total carbon pool in the ocean is the largest reservoir, currently absorbing about 25% of the anthropogenic emissions (http://www.globalcarbonproject.org). Carbon exists in the ocean in many forms (see Table) and spans various spatial and temporal scales. Monitoring the ocean carbon content at the global scale is therefore challenging, as is predicting its fate. In this section, we focus on the assessment of trends in the distribution of the carbon pools and whether they would lead to a possible reduction in strength of the ocean sink in a high CO_2 climate.

The same applies to the carbon pools of inland waters – lakes are reservoirs and regulators of carbon cycling and climate. The amount of carbon processed (sedimentation, outgassing) in inland waters significant despite the relatively small area and volume compared to oceans.

The scientific community represented in GCOS and GOOS has agreed upon a set of Earth observables (named variables) that will contribute to the activities of UNFCCC, IPCC and the monitoring of ocean health status. In particular, phytoplankton biomass, primary production, particulate and dissolved organic carbon have recently been listed as essential ocean variables that should provide feasible long-term information on the role of the ocean as a carbon sink. Satellite remote sensing is the only platform able to provide global-scale estimates of these variables.

Projections of changes in the global carbon cycles and the oceanic sink are made with Earth System Models (ESM), which combine the physical components of climate with the living components that contribute to the fluxes of carbon between the various components within the ocean, and with the atmospheric reservoir. The ocean biogeochemistry models in ESMs now incorporate more sophisticated representations of the biological carbon pump that need to be assessed at the global scale as net production rates and stocks. In addition, all these models have dynamical parameterisations of light acclimation that require independent assessment of the chlorophyll and carbon contents of phytoplankton. All the ESM simulations in the Fifth Climate Model Intercomparison Project (CMIP5) had DOC and POC as state variables, as well as the inorganic carbon components that are central to the solubility of CO_2 in the ocean. Only two out of nine had other components of the carbon cycle, such as bacteria concentration, to resolve the full microbial loop. Many more ESMs will have a complex plankton food web in the next round of the Climate Model Intercomparison Project (CMIP6).

Recommendation: A selected set of gridded global fields will contribute to CMIP6 and to regional and global ocean modelling in general. To maximise the utility, the corresponding fields derived from remote-sensing techniques should be provided at the appropriate temporal and spatial resolutions used by the user community (weekly to monthly resolution, 1 degree WOA grid and 1/4 degree, which are the target grids of most CMIP6 models).

Recommendation: The following fields would greatly benefit the community of Earth System Modellers in CMIP6 and are recommended as priorities:

- Surface and vertically-integrated primary production
- Phytoplankton carbon and distribution of the major PFTs in carbon units
- Total particulate and dissolved carbon pools

Recommendation: Priority should be given to surface fields. It would be desirable to have 3D fields, but this would undoubtedly add considerable uncertainty. The user community would benefit greatly from sensors and products that would provide information on carbon pools and fluxes at higher latitudes, particularly to address the scientific questions on changes in the productivity of polar areas and marginal ice zones.

Finally, according to some primary production comparison projects, the skill associated with primary production estimates by remote sensing is not necessarily superior to that of the forward biogeochemical models.

Recommendation: It is understood that model validation with these remote sensing products is indeed a model-model comparison, but it is nevertheless essential to maintain communication between the two communities and to increase the diversity of approaches. Synergy with observational networks is essential. A related issue is whether we compare like with like when using in situ primary production measurements to assess satellite and numerical model products.

Recommendation: Primary production measured using ^{14}C typically captures only particulate carbon production and may miss a relevant part of carbon production being excreted as DOC. The provision of DOC estimates from remote sensing would greatly contribute to better constraints of these processes. Since most of the biogeochemical models aim at the estimation of net ecosystem production as a proxy to export production, by neglecting this fraction they may underestimate the flow of carbon through the food web.

Recommendation: IPCC and climate modelers need the carbon (mainly DOC) pools in lakes globally only remote sensing can provide. This is important for understanding the role of lakes in the global carbon cycling and parameterizing carbon-climate models. For example, boreal lakes outgas significant portion of carbon fixed by forest around them. This is currently not taken into account.

5.5 Other User Requirements and Technological Opportunities

Numerical models use both nutrients and carbon as currency, and validation of carbon pools in particular is highly desirable. In situ data on carbon pools is extremely limited and even with improved sampling will not have the temporal and spatial coverage achievable from satellite-derived products.

1. It is also desirable to validate long-term trends that are potentially (and uniquely) achievable via merged satellite products.
2. Numerical models may also be developed to assimilate satellite-derived (and other) biogeochemical measurements, as is done currently for physical properties such as SST. Initial attempts to assimilate Chl-a have confirmed that modelled Chl-a fields are thereby improved and also indicate potential avenues for further model development. Continuation along this trajectory would lead to future assimilation of C pools.
3. Validation and/or assimilation of satellite-derived measurements of carbon pools require knowledge of product accuracy and uncertainties (i.e. how close should the model expect to get).
4. Models are applied more and more by user groups including biogeochemical scientists, climate scientists, policy makers, fisheries managers, and carbon products by remote sensing can complement model-derived products.

5.6 Gap Analysis

1. There are differences between modelled properties, and those derived from satellites, that hamper model validation (or potential assimilation). Satellite algorithms and models both include assumptions and methodological differences that may render the products not comparable to each other. The POCO

project has assessed this issue for selected pools. For example, it is not easy to know which model carbon pools (detritus, phytoplankton, zooplankton) should be compared with satellite-derived POC, perhaps estimated from backscattering (and therefore sensitive to small, submicron particles) but validated against in situ POC retained on a particular type of filter (typically, filter that retain particles larger than ~2-7μm).

TABLE 1. The Pools of Carbon in the Ocean

	(carbon units)	**User interest**	**Algorithm available?**	**Validation / maturity level**	**In situ data available?**
DOC	CDOM-DOC	Moderate	Open ocean: No Coastal ocean:: Yes	None Good maturity	DOC:Yes CDOM: Yes Not many combined
	Labile DOC vs refract-tory DOC		unknown		
Particles	Organic	High	Open: Yes Coastal: No	High Low	Yes Yes,but not exploited
	Inorganic	Moderate	Open: Yes Coastal: Yes	High Low/ unknown	Yes Yes
	Living phyto-plankton	Highest	Open: Yes Coastal: No	Low Low	Low Low
	Detritus, including colloidal	Moderate	Open: No Coastal: No		IOP: Yes, carbon:No IOP: Yes Carbon: No
	Other liv-ing: virus, bacteria	Currently Low	Open: No Coastal: No		Unknown

2. Many carbon pools that are resolved in numerical models are not yet derived explicitly from satellites, such as open-ocean DOC and bacteria. In most cases, the limited availability of in situ observations restricts the efforts of modelling and satellite communities.
3. Many carbon pools desired by users are not yet resolved by either satellite or by models, for example, viruses (with few exceptions, ERSEM), and non-organic mineral particles (PIC).

From Table 1, combining the User Requirements with the current knowledge, two further Gaps are revealed:

4. **Recommendation**: Collaboration with modellers (and with observationalists) should continue in the medium and long terms, to develop models and satellite-products that converge and yield the most reliable and robust products for comparison. [i.e. consider where it is ‘best’ to ‘meet in the middle’]. For example, in the case of phytoplankton, comparison of Chl-a from models and satellite are currently considered more robust than comparison between phytoplankton carbon from models and satellite. This is because the Chl-a-to-carbon conversion using mechanistic models is deemed to be more robust than satellite-derived phytoplankton carbon products available now. But model-generated phytoplankton carbon fields are rarely validated extensively, and so there is possibility for improvement there as well. Both models and satellite products of phytoplankton carbon need improvements, and would benefit from comparisons and interactions.
5. Models differentiate many components of particulate carbon pools, such as living+dead particles, all particles and particles delimited by size, for which there may not be a comparable satellite product. So model-satellite products are at present limited to total particulate carbon pools rather than the components.
6. Models can help inform satellite algorithm development, as well as identify locations or conditions for in situ sampling (already started in POCO).
7. DOC: There are no available algorithms for the open ocean, because CDOM is not directly related to DOC in the surface, but there is potential for exploiting other optical properties at different wavelengths (UV). This is limited by non-availability of EO at the appropriate wavelengths.

8. POC: In the open ocean, empirical POC algorithms have reached maturity, but mechanistic options are preferred. In coastal/inland waters there are no algorithms available currently, but the interest of the community is high.
9. **Recommendation:** Both models and satellite products suffer from lack of sufficient in situ data for validation, and so a rigorous in situ observation programme is essential for further development of both models and satellite algorithms for pools of carbon. In some instances, methodological developments are necessary for routine in situ measurements of certain pools, such as phytoplankton carbon pool, which is extremely difficult to measure in situ

5.7 Organic matter in the ocean

Organic matter can be considered as a frontier topic under the CLEO umbrella. This section presents a discussion with particular focus on this topic.

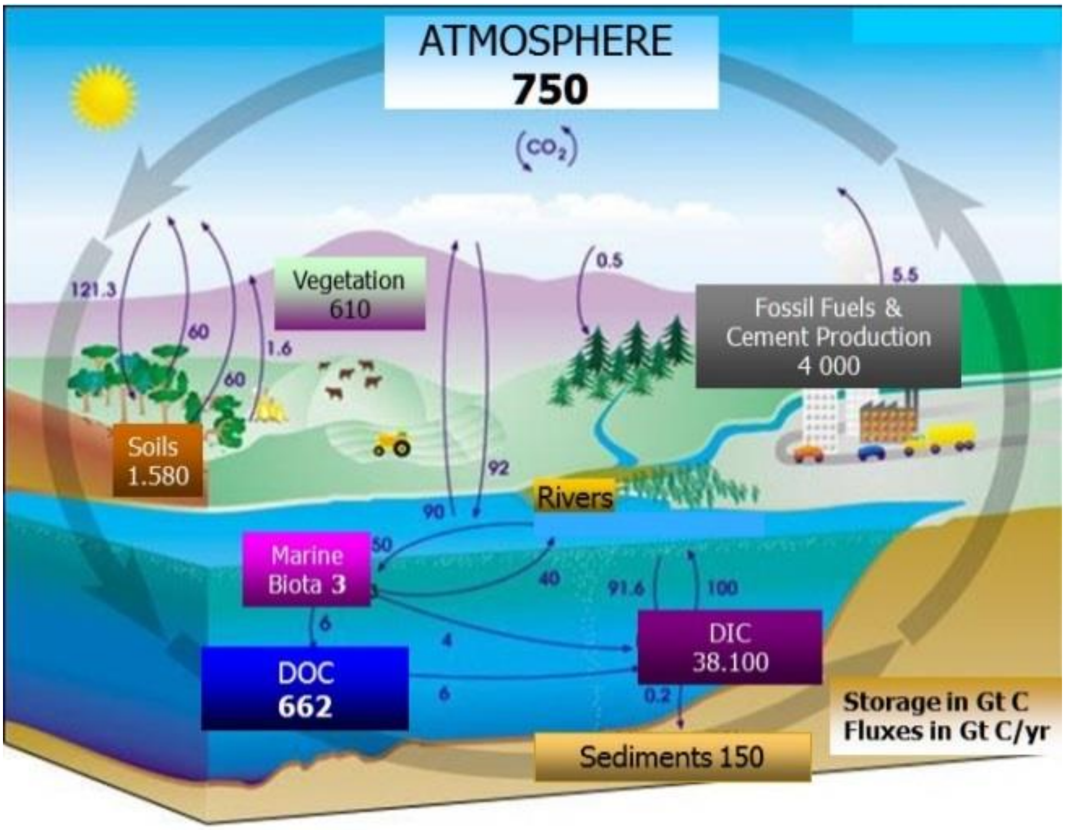

Figure 1:
In OM, pool two fractions can be operationally defined: the particulate organic carbon (POC) that is retained by a GF/F filter, and the dissolved organic carbon (DOC), that passes through a 0.2 µM filter (Fig. 2). Adapted from a Schematic representation of the global carbon cycle http://earthobservatory.nasa.gov/Library/CarbonCycle/carbon_cycle4.html.

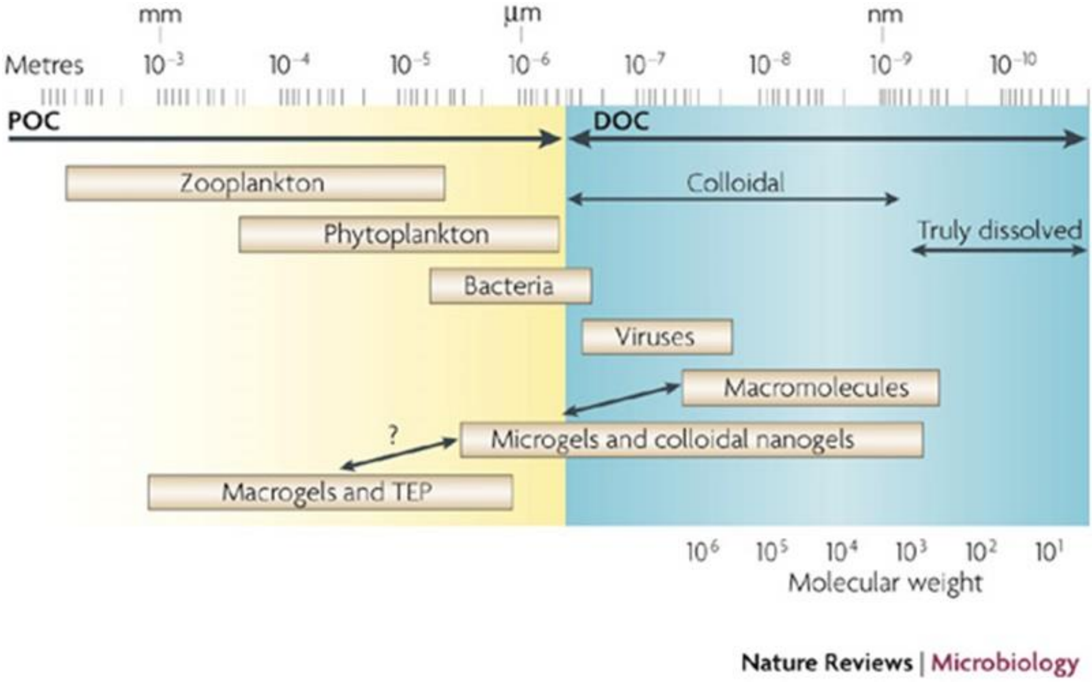

Figure 2: Full size range of organic matter from monomers to traditional particles. The separation between particulate organic carbon (POC) and dissolved organic carbon (DOC) is clearly indicated. From Azam and Malfatti (2007).

Organic matter in the oceans (OM) represents the largest, most complex, and least understood reservoir of organic carbon on the Earth. Its importance is connected to its ecological significance and its central role in the carbon cycle (Fig. 1). It is produced at all the levels of the food web and its oxidation is responsible for considerable consumption of oxygen. Respiration is therefore tightly coupled to organic matter removal. Understanding the OM cycle, as well as its response to global change, is one of the most pressing and fascinating issues in marine science.

Particulate Organic Carbon (POC)

POC in the surface ocean may represent up to 10% of OM. It includes autotrophic and heterotrophic organisms and biogenic detrital particles. Sinking of POC from surface waters is part of the biological pump that provides a mechanism for storing carbon in the deep ocean, a long-term sink for atmospheric CO_2 (Stramski et al., 2008). It used to be thought that transport of POM to bottom waters was mostly confined to large, rapidly-sinking fecal pellets. However, recent studies have highlighted the importance of organic aggregates and flocs, formed by diatoms such as *Rhizosolenia* and other microalgae, in C export to depth. Ascending particles have also been discovered, many of which are lipid-rich (Volkman and Tanoue, 2002). Knowledge of total POC concentration and subsequent inference of the phytoplankton portion of POC is essential to the development of methods for estimating phytoplankton growth rates and carbon-based net primary production from satellite observations (Behrenfeld et al., 2005; Sathyendranath et al. 2009).

Recommendation: Because the turnover time of carbon biomass is relatively short (1–2 weeks), satellite capabilities to monitor changes in particulate carbon pools can effectively aid in studies related to the biological pump (Stramski et al., 2008).

Dissolved Organic Carbon (DOC)

DOC (>90% OM) contains an amount of C comparable to that occurring in the atmosphere as CO_2. As a consequence, the net oxidation of just 1% of its pool would introduce to the atmosphere an amount of CO_2 commensurate with that released by the fossil fuel burning in one year (Fig. 1). DOC also represents the main source of energy for heterotrophic prokaryotes fueling the microbial loop. Depending on the growth efficiency of heterotrophic prokaryotes and their grazers, the microbial loop can represent a link of C to the food web, channeling the energy towards higher trophic levels, or a sink of C, transforming most of DOC into CO_2 and inorganic nutrients. This scenario is further complicated by viral lysis of prokaryotes (a part of POC) that acts to convert most of the energy from POC to DOC (Carlson and Hansell, 2015). DOC plays a crucial role in C export and sequestration to depth by deep-water formation and winter mixing (Carlson and Hansell, 2015; Santinelli, 2015). DOC includes molecules with a wide range of biological lability; different fractions have been described in its pool, based on their turn-over time. Labile DOC (LDOC) is used immediately by heterotrophic prokaryotes and does not, by definition, accumulate. DOC that does accumulate is considered to be recalcitrant; at least four fractions have been distinguished depending on their lifetimes: semi-labile DOC (SLDOC, lifetime ~1.5 years), semi-refractory DOC (SRDOC, lifetime ~20 years), refractory DOC (RDOC, lifetime 16,000 years) and ultra-refractory DOC (URDOC, lifetime ~40,000 years) (Hansell, 2013). SLDOC plays the most important role from both an ecological and a biogeochemical perspective. Recently, it has been proposed that fluorescent dissolved organic matter (FDOM) could be a tracer for RDOC. External sources (atmosphere, rivers, groundwater and sediments) strongly affect DOC concentration and distribution (Carlson and Hansell, 2015). Atmosphere and rivers are also a source of pollutants to the ocean, organic pollutants will therefore represent an important fraction of allochthonous DOC.

CDOM (Coloured Dissolved Organic Matter)

The fraction of DOM capable of absorbing light (PAR, UV-A and UV-B) is defined as chromophoric or coloured DOM (CDOM). Also known as yellow substance, humic color, and gelbstoff, CDOM is an important measure of water quality and has important implications for aquatic ecosystems (Häder et al., 2007) and metal transport (Bergamaschi et al., 2011). A fraction of CDOM, defined as Fluorescent DOM (FDOM) can emit the absorbed light. CDOM determines the underwater light availability in the open ocean and coastal waters. Functionally, CDOM can have a contrasting effect: it can protect organisms from ultraviolet radiation in the upper layer, but it can also reduce the visible light, limiting photosynthesis (Häder et al., 2007). Although naturally occurring, CDOM can also be increased by anthropogenic activities such as agricultural runoff, sewage treatment plant discharge, and runoff from confined animal feeding operations as well as by extreme weather events, such as storms and hurricanes, causing massive overland flow and washing of surface material into estuarine waters (Hudson et al., 2007). The enhancement of UV-B radiation reaching the Earth induces photochemical reactions that affect the quality and the quantity of CDOM in the upper layer of the water column, with important implications for the CO_2 flux from the sea surface to the atmosphere.

Recommendation: CDOM is optically measurable and therefore an excellent candidate for quantification by remote sensing techniques. Understanding the spatial and temporal variability of CDOM is important to the study of water quality, global carbon budgets, and climate change (Slonecker et al., 2016).

Organic Matter (OM) and Good Environmental Status (GES)

Due to the strict link between ecosystem functioning and DOC/POC dynamics, Good Environmental Status (GES) is strictly linked to OM cycle, in synthesis:

- Anomalous DOC concentration in open sea waters (<34 or >100 μM) is indicative of perturbation of marine ecosystem function.
- OM interacts with metals, contaminants and nanoparticles, changing their bioavailability.
- Photodegradation of CDOM can release CO, CO_2 and free radicals dangerous for organisms.
- OM includes in its pool organic contaminants. Most of them absorb light, they can be therefore be traced by using CDOM/FDOM.
- High input of OM in coastal water can lead to eutrophication and anoxia.
- Large amounts of preformed OM in deep water can lead to high oxygen consumption in deep waters with consequent hypoxia and/or anoxia.

Importance of satellite retrieval of OM pools

POC, DOC and CDOM cycles are very complex and show seasonal and interannual variability. Up-to-date information on OM is gained mostly by in situ sampling and laboratory analysis. This approach, expensive and time-consuming, cannot give a synoptic view of OM distribution at large scale nor accurate information on its temporal variability. This is even more important in coastal areas where terrestrial inputs are crucial in closing carbon budgets, but they are also very variable in both space and time.

Recommendation: Satellite retrieval should be developed to help to fill many of the gaps in our knowledge of the distribution of, and variability in, POC, DOC and CDOM; it could provide an accurate estimate of their fluxes from the land, as well as information about their spatial and temporal variability both in coastal and open sea areas (for the moment just for POC and CDOM).

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5.8 Research and Development Priorities for Carbon Pools and Fluxes

Priority variables

Dissolved organic carbon

Absorption by coloured dissolved organic matter is retrievable from satellite ocean colour as a standard product (e.g. within OC-CCI, and from NASA). There is a gap in quantifying this product in carbon units (CDOM is usually reported as an absorption coefficient). Algorithms have been proposed to estimate DOC in carbon units in coastal and inland waters, however limitations include: seasonal and regional variability in empirical relationships, and difficulty to extend to an open ocean application.

Priorities in this area would be:

Recommendation: Establish an algorithm development data set covering a variety of global water types including simultaneous measurements of optical properties and DOC.

Recommendation: Investigate the dependencies of the CDOM-DOC relationship, to enable translation of CDOM absorption (currently available from satellites) into carbon units more useful in bio-geochemical studies.

Recommendation: Explore the potential application of fluorescence techniques for estimating DOC from hyperspectral sensors and/or LIDAR techniques. Sensitivity and feasibility studies would have to be undertaken to establish whether or not such a mission would be justifiable.

Dissolved inorganic carbon

Dissolved Inorganic Carbon (DIC) is the largest carbon pool (38,000 Pg of carbon) in the ocean, and plays a key role in the solubility pump; it is therefore of relevance to both ocean carbon dioxide uptake and ocean acidification. While recognising the importance of this pool, the CLEO workshop did not discuss the inorganic carbon pool in great detail. We anticipate that the Ocean Fluxes Meeting (Oceanflux Greenhouse Gases Evolution Project led by Dr. Jamie Shutler), occurring simultaneously in Brest would have addressed this adequately. Furthermore, some of the methods that have been developed for estimation of components of the DIC pool (e.g. alkalinity) are based on satellite inputs other than ocean colour, and therefore fell outside of the scope of the CLEO workshop. To quantify the partitioning of DIC (e.g. into dissolved CO2, carbonic acid, bicarbonate, carbonate) requires four measurements: Total Inorganic Carbon, pH, Alkalinity and Partial Pressure of CO2.

Recommendation: Encourage further developments of DIC-related algorithms from satellites, combining, as needed, ocean-colour, salinity and sea surface temperature.

Particulate carbon

The particulate carbon pool was discussed substantially at the CLEO workshop, and the importance of partitioning the pool into its components was highlighted. The R&D priorities for each of these components are listed next.

The total particulate organic carbon pool:

Participants agreed that algorithms were most advanced for detection of total POC.

Recommendation: The following priorities were identified:

a) Characterise the composition and structure of the POC pool e.g. type (phytoplankton, detritus, bacteria), size structure (<1nm to >1mm).

b) Improve algorithm performance in coastal and inland water bodies.

Avenues to achieve these targets include:

a) Development of reflectance models, taking into account inherent optical properties of POC, and sensitivity studies to establish algorithm feasibility.

b) Optical classification of waters according to the composition of POC.

c) Algorithms tuned to particular compositions of POC/optical classes.

Phytoplankton Carbon pool:

This pool is of particular interest to the user community. The algorithms for quantification of the phytoplankton carbon pool have not reached the same level of maturity as those for the POC algorithms. Challenges include: high dynamic range in the C:Chl ratio, absence of an identified optical signature that can be used to separate phytoplankton carbon from other types of particulate carbon, dynamic variability in the detritus-carbon-to- phytoplankton-carbon ratio, and the discrepancy between the operational definitions of phytoplankton carbon derived in situ versus that derived from satellite.

Recommendation: Many of the priorities described above for addressing the particulate organic carbon pool will be of benefit for deriving phytoplankton carbon also (i.e characterisation of size structure and relationships to optical parameters).

Recommendation: This particular pool also requires consideration of physiological factors such as photoacclimation. Progress will require close collaboration between remote-sensing scientists, the modelling community (especially physiological models) and in situ observations.

Recommendation: A workshop of experts will be useful to bring consistency and standardisation in in situ measurement methods and to establish how these might be related to optical signals (for example, on a cell size/functional type/physiological basis).

Recommendation: Since carbon content per cell varies with cell size and with phytoplankton type, this line of research would benefit from hyperspectral and LIDAR missions, for detection of fluorescence signals and different types of phytoplankton.

Other carbon components

Several components of the carbon pools were identified as being understudied, with relatively immature approaches for defining them from space. These components were nevertheless important to the user community and warrant explorative studies on the feasibility of their detection from space. The workshop discussion did not cover particulate inorganic carbon (PIC) in great deal. The discussion acknowledged the progress made on quantification of biologically produced PIC (e.g. algorithms to detect coccolithophore produced PIC). There is a lack of algorithms to quantify non-biological PIC, which can influence biogeochemically-important processes including light limitation, ballasting, and nutrient provision. It is expected that work to characterise particulate assemblages would help in development of algorithms for this purpose.

Recommendation: Further work needs to be done on the potential for detection of other components of carbon pools with important biological functions, such as colloids and other living components such as viruses, bacteria, and zooplankton.

Fluxes

Due to links with the "Pools of Carbon in the Ocean" Project, a primary focus of the CLEO workshop was pools of carbon rather than fluxes between these pools, or fluxes between the air and sea, or within the sea (such as export from the surface to deep ocean). However, the workshop included presentations from projects dealing with primary production, an important flux that can be determined both from satellite and biogeochemical modelling methods. Further focus is required on the derivation and validation of primary production parameters from space, round robin method comparisons between satellites and models. Similarly, other fluxes with the potential to be derived from satellite (e.g. those considered under the Oceanflux Greenhouse Gases Evolution project) should be assessed. It is recommended to develop opportunities for these fluxes to be discussed, particularly in the context of how they may utilise estimates of carbon pools, or be used by the modelling community.

Summary of suggested activities to meet short–term requirements:

1. Establish consistent definitions of carbon pools and components across in situ, satellite and modelling techniques.
2. Develop measurement protocols for *in situ* variables and incorporate the routine collection of these into satellite validation planning across agencies and institutions.
3. Conduct sensitivity studies to determine how characteristics of carbon pool components are represented optically.
4. Classify water types according to their carbon pool characteristics.
5. Use these classifications to develop, select, and blend algorithm approaches for optimal products.
6. Inclusion of mature products (such as POC) into Essential Climate Variable programmes, such as any further developments of the OC-CCI project.
7. Provision of toolboxes
8. Delivery of such products to the user community in the formats required i.e. on suitable grids for model validation/assimilation. Alternatively, provision in toolboxes for transforming products for this purpose.
9. Studies to develop quantification of uncertainties for satellite carbon products.
10. Organise further workshops to aid in meeting the above goals and continue valuable interaction between ESA, satellite remote sensing.

Longer–term requirements

11. Input findings from sensitivity studies to the design of new satellite sensors e.g. addition of specific wavelengths, selection of hyperspectral/geostationary sensors.
12. Communication with satellite and model communities to develop both approaches in a way that improves ability to compare like for like.

Acronyms Used in the Report:

AOP = apparent optical property
chl-a = chlorophyll *a* concentration
CCI = Climate Change Initiative
CDOM = coloured dissolved organic matter
conc. = concentration
CPR = Continuous Plankton Counter
DOAS = Differential Optical Absorption Spectroscopy
ECV = Essential Climate Variable
EnMAP= Environmental Mapping and Analysis Program mission
Envisat = Environmental Satellite
EO = Earth Observation
HABs = Harmful Algal Blooms
HICO = Hyperspectral Imager for the Coastal Ocean
HPLC = High–Performance Liquid Chromatography
HyspIRI = nHyperspectral Infrared Imager
IOCCG = International Ocean Colour Coordinating Group
IOP = inherent optical property
MERIS = Medium Resolution Imaging Spectrometer
MODIS = Moderate Resolution Imaging Spectroradiometer
MSI = MultiSpectral Instrument
OC = Ocean Colour
OC-CCI = Ocean Colour Climate Change Initiative
OC-PFT = Algorithm of Hirata et al. (2011)
OLCI = Ocean Land Colour Imager
OMI = Ozone Monitoring Instrument
PACE = Pre-Aerosol, Clouds, and ocean Ecosystem
PhytoDOAS = DOAS applied for retrieval of phytoplankton biomass (PFT algorithm by Bracher et al. 2009, Sadeghi et al. 2012)
PFT = phytoplankton functional type
PG = phytoplankton group
PSC = phytoplankton size class
PT = phytoplankton type
S = Sentinel
SCIAMACHY = Scanning Imaging Absorption Spectrometers for Atmospheric Chartography
SeaWiFS = Sea-viewing Wide Field-of-view Sensor
SEOM = Scientific Exploitation of Operational Missions
TropOMI = TROPOspheric Monitoring Instrument
TSM = total suspended matter
UVN = Ultra-violet/Visible/Near-Infrared Instrument
WG = Working Group