Report on Challenges, Gaps, and Opportunities based on the Particulate Organic Carbon session at the Carbon From Space 2022 Workshop
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Topical area #1: POC measurement methodology

Challenges:

The current filtration-based methodology that uses glass-fiber filters for retaining particles and measuring POC does *not* include all POC-bearing particles, and hence does *not* determine the total POC. In particular, some fraction of submicrometer POC-bearing particles is missed by this method. Other sources of possible underestimation of total POC include the loss of POC due to the impact of pressure differential across the filters and underrepresentation of contribution of relatively rare large particles associated with a limited filtration volume.

The optical remote sensing including ocean color measurements from space are driven by *all* particles suspended in water, including particles which are missed and/or underrepresented by the current filtration-based POC methodology. Thus, there is a mismatch between POC and optical measurements that serve as a predictor of POC. The missing portion of POC unaccounted for by the current filtration-based POC methodology is important to both the ocean biogeochemistry and ocean optics underlying ocean color measurements from space.

While standardization of POC methodology is generally desirable, there are important interpretive challenges that must be recognized in the course of standardization process. In particular, while the recommendation to use DOC-adsorption correction in the standard filtration-based method will result in correction for one known source of overestimation of the fraction of total POC that is strictly retainable on the filters (IOCCG Protocol Series, 2021), the issue of known sources of underestimation of total POC remain unresolved. Thus, while the use of DOC correction alone is expected to improve the estimate of POC that is strictly retainable on the filters, such DOC-corrected measurement without parallel correction for the sources of POC underestimation is likely to provide an inferior estimate of total POC compared with the measurement without DOC correction.

The fractional contributions to POC associated with differently-sized particles and/or different types of particles (e.g., different groups or species of microorganisms) are difficult to quantify and remain poorly known for natural polydisperse and heterogenous assemblages of suspended particles.

Gaps:

The current standard POC method based on the analysis of particles retained on filters (most commonly GF/F glass-fiber filters) does *not* quantify the total POC because some POC-bearing particles (primarily submicrometer particles) pass through the filters, some portion of POC can be drawn through the filter under pressure differential, and relatively rare large particles can be underrepresented by the sample volume. The current standard method does *not* account for both the artificial gains and losses of POC during collection of particles by filtration. No experimental capabilities exist to partition total POC of natural particulate assemblages into contributions by different size fractions and/or different types of particles which play different roles in ocean biogeochemistry and carbon cycling.

Opportunities:

Advance and standardize measurement methodology to provide improved estimates of total POC. These advancements can be brought about by including the portion of POC that is unaccounted for by the current standard filtration-based method. Develop measurement capabilities aiming at quantification of POC contributions associated with differently-sized particles and different particle types based on combination of single-particle measurement techniques for particle sizing, particle identification, and particle optical properties.

Topical area #2: Data

Challenges:

The POC algorithm development and validation depend on datasets used in these analyses. For the purposes of algorithm development or validation, the field-based datasets are commonly compiled from data collected by different investigators on many oceanographic expeditions covering a long period of time. The information content available in documentation of various individual datasets is non-uniform and does not always contain sufficient details about data acquisition and processing methodology. This creates a risk that the compiled datasets are affected by methodological inconsistencies across diverse subsets of data, including the potential presence of methodological bias in some data. The presence of methodological bias is generally difficult to identify given the range of environmental variability, especially when available details on data acquisition methods are limited and/or there is a lack of replicate measurements. Thus, indiscriminate use of data for the algorithm development and validation analyses is not advisable. These issues pose significant challenges for assembling high-quality field datasets that meet the objectives of algorithm development or validation analyses including, for example, the process of data quality control based on predefined set of inclusion and exclusion criteria and assurance of environmental representativeness of datasets assembled for the analysis of specific algorithms (e.g., global vs. regional).

The common validation strategy that relies on comparisons of field-satellite data matchups is not solely sufficient to ensure rigorous assessment and understanding of various sources of uncertainties in satellite-derived POC product. The deviations between field and satellite data matchups can occur for various reasons such as spatiotemporal mismatch of data, uncertainties in both satellite and in situ measurements, atmospheric correction, and performance skills of the in-water algorithm itself. In addition, the number of available data matchups is often limited in various environments.

Gaps:

While the documentation of data acquisition and processing methods is often limited, especially in historical datasets, there are no standardized best-practice guidelines to ensure consistency in data quality control and synthesis efforts when larger datasets are compiled from various individual subsets of data.

There are regions within the world's oceans, such as polar regions and the Indian Ocean, where concurrently collected field data of POC and optical properties are very scarce or non-existent including the lack of temporal coverage over the entire seasonal cycle.

Opportunities:

Further efforts related to POC algorithm development and validation can benefit from careful scrutiny of historical and future data to minimize the risk of using biased data and ensure that the analyses are conducted using data with consistently high quality and are accompanied with sufficiently detailed documentation on data acquisition and processing methods. These efforts can be facilitated through further improvements and standardization of best practices for documentation, quality control, sharing, and submission of data into database archives. Such practices are expected to lead to better data quality, data interpretation, and uncertainty assessments.

There is a need to continue field programs in which concurrent POC and optical data are acquired across diverse environments including those that have been severely undersampled in the past. This task can benefit from a widespread use of autonomous observation platforms, which should also be accompanied by improved data quality control procedures.

Topical area #3: Satellite retrievals

Challenges:

High level of complexity and variability of water optical properties and water constituent composition including POC-bearing particles, especially in coastal regions and inland waters which are highly susceptible to land effects and re-suspension of sediments from shallow bottom, makes it very difficult to develop a unified approach to provide reliable POC retrievals from optical remote sensing along the continuum of diverse optical/biogeochemical environments from open ocean to coastal and inland water bodies.

The current standard global POC product is generated indiscriminately with respect to optical water types or optically significant composition of water. Hence, this product is generated for a wide range of environmental situations, including the conditions outside the intended scope of global algorithms which implies unknown and potentially large uncertainties.

The satellite inter-mission consistency of POC product is required in support of long-term climate data record.

Gaps:

The current routine process of generating standard global POC product from global empirical algorithms lacks the mechanistically-based flags associated with ocean properties or optical water types to prevent the application of algorithms beyond their intended use and minimize the risk of generating the product with unknown large uncertainty (e.g., optically complex waters with mineral-dominated particulate assemblages). The need for appropriate flags to prevent the use of algorithms outside their scope is broadly relevant, for example it applies also to regional algorithms.

There is a lack of advanced algorithms based on adaptive approaches that incorporate mechanistic principles of interaction and light and water constituents and associated optical water typologies. For example, algorithms that discriminate the water bodies based on varying composition of organic and mineral particles are required to enable reliable POC retrievals across diverse environments including the optically-complex coastal water bodies.

Opportunities:

Recent development of a new suite of empirical satellite sensor-specific global POC algorithms provide the opportunity for further testing, validation, analysis of inter-mission consistency, and ultimately an implementation of next-generation algorithms for routine production of refined global POC product.

Development of new algorithmic approaches with enhancements offered by potential incorporation of mechanistic principles underlying interactions of light with water constituents will support and advance future remote sensing applications along the continuum of diverse aquatic environments.

The analysis of POC reservoir and its spatiotemporal dynamics is expected to be enhanced by increased availability and use of satellite geostationary and hyperspectral data along with in situ data.

Topical area #4: Partitioning of POC into distinct components by biogeochemical function and/or size

Challenges:

One of the most challenging, yet important tasks moving forward is to develop understanding of the different functional and/or size partitions of POC. Bulk POC does not give a full picture of the ecosystem or its biogeochemical role, e.g., for the biological pump. In addition, empirical POC satellite algorithms rely on certain relationships between POC and optical properties. These relationships can change if basic characteristics of the POC change, e.g., its PSD or the fraction of total POC due to living phytoplankton. For example, the POC-specific backscattering coefficient can change if the PSD of POC changes, and the POC-specific absorption spectra can change if the living C:POC ratio changes.

Notwithstanding the operational limitations of what constitutes POC vs. dissolved substances within the submicrometer size range, the particle assemblages in the near surface ocean are exceedingly complex, which makes this challenge particularly difficult to address. In addition, both forward and inverse modeling of the optical properties of the ocean entirely from first principles are infeasible. The range from truly dissolved substances to particles such as large zooplankton and beyond span many orders of magnitude in size and are governed by different optical regimes, which makes it difficult, for example, to identify, quantify, and separate the various sources of optical backscattering in the ocean.

In terms of functional fractions, POC can be considered to consist of phytoplankton, heterotrophic bacteria, zooplankton, and organic detritus. In terms of size fractions, ideally the PSD of POC and its various functional components should be measured in-situ. The PSD is an important link between ecosystem structure and function on the one hand, and optical properties on the other, as it affects both. There are theoretical considerations indicating that the marine bulk PSD spanning many orders of magnitude in size approximately follows a power-law of certain slopes. Phytoplankton cell size is a master trait, and size fractions are closely related to functional types.

Finally, optically complex coastal waters present an additional challenge in that allochthonous and autochthonous sources of POC may be mixed, e.g., due to riverine input, making the task of separating POC by functional fractions with known or assumed optical properties or PSD more challenging.

Gaps:

Dearth of PSD and phytoplankton carbon (phyto C) data sets is a major limiting factor for satellite algorithm development.

Opportunities:

Efforts must be directed toward progress in this area, including basic research to enable us to exploit upcoming hyperspectral and polarization remote-sensing data. It is important to emphasize measurement of PSD in future field campaigns globally, and the compilation of global, quality-controlled data sets for algorithm development.

Topical area #5: Vertical profiles of POC

Challenges:

Whereas vertical profiles of POC can be estimated from in situ optical sensors (in particular, backscattering sensors and transmissometers) deployed on autonomous in situ platforms, the performance of present optical-based POC algorithms is hampered by limited understanding and predictability of variations in the characteristics of particulate assemblages and their relationships with optical properties throughout the water column.

Gaps:

One of the most frequently asked questions posed by users of ocean color remote sensing data (e.g., modelers) is what the satellite sensor actually "sees", in particular how deep the satellite sensor probes the water column in terms of variable near-surface vertical profiles of retrieved data products such as POC.

Opportunities:

Further research is needed to improve an understanding between POC and optical properties that are potentially amenable to measurements from autonomous in situ platforms such as Biogeochemical Argo floats. Such research is expected to guide development of new sensors and algorithms (e.g., scattering sensors that include polarization) which will ultimately provide more reliable estimations of POC throughout the water column from autonomous systems.

More emphasis is required to highlight the need and promote more basic research to better quantify and understand the relationships between variable vertical profiles of POC (and characteristics of the POC such as PSD, functional and size fractions) and the optical signal detectable from satellites.

Due to the double trip light has to take through the water column between the ocean surface and a given depth (downwelling radiance and then upwelling radiance), the source of the water-leaving optical signal reaching the satellite is heavily weighted to the near-surface layers of the ocean. Early research from the 1970s demonstrated that ~90% of the water-leaving signal comes from an e-folding attenuation depth, i.e., the layer defined by 1/Kd, where Kd is the wavelength-dependent diffuse attenuation coefficient for downwelling irradiance. There is a need to expand on this research and develop POC-specific understanding, including the effects of vertical profiles of variables going beyond just bulk POC, namely POC partitioned by functional and/or size fractions (see Topical Area #4). The diurnal evolution of the characteristics of POC vertical profiles also needs to be taken into account.

Topical area #6: Biogeochemical processes and the biological carbon pump

Challenges:

The biological carbon pump (BCP) is a process whereby the CO_2 fixed by primary producers in the upper ocean is transported to the deep ocean. This process influences climate because it regulates the oceans' capacity to store atmospheric carbon over centennial to millennial time scales. It is estimated that around 80% of the carbon is exported in the form of POC, and the remainder is transported downward as DOC via vertical mixing and advection.

The vertical export of POC results from several biological and physical processes, of which gravitational POC sinking is the largest component. Gravitational sinking speed is a function of particle size, composition, and structure. The distribution of these properties in the particle population results to a large extent from the functioning of the upper-ocean ecosystem. Therefore, improving the satellite retrieval of POC mass (Topical Area #3), size distribution (Topical Area #4), and vertical distribution (Topical Area #5), as well as additional particle properties (e.g. composition), is key to understanding and predicting the operation of the BCP at various scales.

Quantifying the global vertical POC export flux is a major challenge, as the range of current estimates (ca. 5–15 Pg C yr^{-1}) has not narrowed down significantly compared to the ranges quoted in the 1980s. Improved ability to estimate the concentration and fluxes of POC would also benefit the study of trace element cycling and deep-ocean ecosystems that rely on vertical organic C fluxes. However, current methods to measure gravitational POC export are work-intensive and do not allow for high spatiotemporal coverage. Moreover, they often rely on simplifying assumptions (steady-state vertical profiles, negligible effects of horizontal advection, to number just a few) whose validity is not always tested or subjected to sensitivity analyses. Therefore, empirical (e.g., remote-sensing based) and prognostic models of gravitational POC export rely on in situ measurements that are inherently uncertain and have sparse spatiotemporal coverage.

Gaps:

The relationship between upper-ocean biogeochemical properties and vertical POC fluxes is still very uncertain, which hampers their representation in empirical and mechanistic models of the BCP. Large-scale estimates of vertical POC export usually focus on the average (climatological) state of the ocean, but interannual variations and their drivers (e.g. the role of physical forcing) remain poorly known, and because of data sparseness there is a risk of confounding spatial and temporal variability.

Although shallow seas and continental slope areas are thought to play an important role in the global POC cycle, the sources and fate of POC in these areas remain difficult to monitor and quantify owing to the presence of optically complex environments, the higher abundance of inorganic particulate materials and the potentially larger role of lateral advection.

Opportunities:

Sampling from autonomous platforms (biogeochemical Argo, gliders, moorings, etc.) can provide the spatial-temporal resolution needed to refine our understanding of the BCP, complementing more detailed shipborne observations and the synoptic surface view obtained from satellites. For example, "optical sediment traps" mounted on biogeochemical Argo floats can record a nearly-continuous proxy of vertical POC fluxes in the ocean interior.

Merging of these various data streams via statistical techniques, e.g. machine learning, can allow for refined estimates of the BCP, reducing the sampling bias associated with shipborne measurements. These complementary data streams can be further used to constrain mechanistic models of the BCP, for example through data assimilation and parameter optimization. These approaches will improve quantification of the fluxes that form the BCP, help identify knowledge gaps and eventually spur progress in process-level understanding.

Although the framework drafted above is conceptually valid for the study of continental shelves, these areas require higher-resolution observations and models that can resolve their larger heterogeneity and a wider array of transport and transformation processes. Therefore, such areas would benefit from dedicated regional process studies and monitoring from geostationary satellites and other airborne sensors.

POC	Challenges	Gaps	Opportunities
Measurement methods	• Inclusion of particles of all sizes to determine total POC • Quantifying contributions of differently-sized particles and different particle types	• Submicrometer particles missed and rare large particles potentially underrepresented in the standard filtration method • No capability to measure contributions of differently-sized particles and different particle types	• Advance and standardize methods for improved measurement of total POC • Develop measurement capabilities combining particle sizing, particle identification, and particle optical properties to address contributions of different particle sizes and types
Data	• Quality control and consistency across diverse datasets • Limitations of satellite-in situ data matchups, e.g., spatiotemporal scale mismatch, availability of matchups in various environments	• Limitations in documentation of methods in historical datasets • Best-practice guidelines for data quality control and synthesis efforts • Undersampled environments	• Improve and standardize best practices for documentation, quality control, sharing, and submission of data into permanent archives • Collection of high-quality data along the continuum of diverse environments
Satellite retrievals	• Unified algorithms for reliable retrievals along the continuum of diverse aquatic environments ranging from open ocean to coastal and inland water bodies • Global algorithms applied to environmental conditions outside the intended scope • Satellite inter-mission consistency	• Mechanistically-based flags associated with optical water types to ensure the application of algorithms (e.g., the current global algorithms) according to their intended use • Advanced algorithms (e.g., adaptive algorithms based on mechanistic principles) to enable reliable retrievals across diverse environments including the optically-complex coastal water bodies	• Recent development of a new suite of empirical satellite sensor-specific global POC algorithms provides the opportunity for routine production of refined global POC product • Development of advanced algorithms that incorporate mechanistic principles for applications across the continuum of diverse aquatic environments • Use of satellite geostationary and hyperspectral data in combination with in situ data

Functional fractions	• Partitioning of POC into particle size fractions and biogeochemically important components • Characterize the PSD of both total bulk particle assemblages and separately the various functional fractions • Address coastal and other optically complex water bodies that may have both autochthonous and allochthonous contributions to POC, as opposed to dominance of autochthonous POC in the open ocean - assess the need to separate these two pools	• Ability to reliably measure in-situ various fractions is limited, e.g. separate living vs. non-living POC • Insufficient global PSD measurements and lack of comprehensive global PSD data compilations • Insufficient knowledge of IOPs (e.g., VSF) for optics-based paritioning of POC	• Support basic research on particle sizing, particle identification, and particle optical properties including polarization properties • Development of light-scattering polarization sensors for deployment on autonomous in situ platforms (in combination with other IOP sensors such as cp and bbp) • Emerging techniques to separate living vs. non-living POC. • Support PSD measurements as part of a suite of basic required variables for ocean biogeochemistry studies and remote sensing
Vertical dimension	• Reconstructing vertical profiles using data from space-borne, air-borne, and in-situ sensors • Determining relationship(s) between remotely-sensed variables and characteristics of POC vertical profile, e.g. weighted average	• Relationships between optical variables and POC (e.g., from sensors on autonomous in situ platforms) - also see notes above on functional fractions	• Development of POC algorithms for in situ optical data (e.g., BGC-Argo) along with improvements of optical sensor technology (e.g., polarized scattering sensors for BGC-Argo) • Use multiple data (satellite, BGC-Argo) and model streams (including CMIP6 ocean bgc models) to reconstruct 3D and 4D POC in the ocean via statistical and data assimilation techniques • Advance basic research to determine relationships between remote-sensing reflectance and other optical variables and vertical profiles of POC characteristics, including PSD and functional fractions

Biogeoche-mical processes and carbon pump	• Understand the fate of POC and its fractions globally, e.g., the role of POC in the biological pump	• Interannual POC export variability in empirical and mechanistic models • Fate of POC in shallow environments • Role of horizontal advection	• Widespread use of autonomous sensors and emerging observation techniques (e.g., “optical sediment traps” on BGC-Argo floats) • Data-driven estimates of vertical POC fluxes • Constraining prognostic ocean BGC models using observations from remote and in situ autonomous sensors