

Ocean Ecosystems and Biogeochemistry Measurement Requirements

The introductory section on PACE Ocean Ecology and Biogeochemistry identifies seven overarching Science Questions and associates each of these questions to a specific set of geophysical properties or processes. These sets of science-driven property retrievals define measurement requirements that exceed those of heritage sensors, particularly in terms of measurement spectral range and resolution. PACE science objectives also extend from near-shore waters to the broad open ocean, which has implications on desired spatial resolution. Multiple aspects of the PACE Science Questions are also several steps removed from the primary observations of the PACE ocean radiometer and thus require additional inputs from contemporaneous operational satellites, *in situ* oceanographic and atmospheric observations, and significant integration of PACE data into Earth System models. The Ocean Ecology and Biogeochemistry introduction also describes PACE approaches for achieving its science goals through retrievals of essential ocean ecosystem and biogeochemical properties (**subsections i – xv**), including a mapping of measurement spectral bands to specific retrieved properties.

In this section, a detailed description is provided of science-driven measurement requirements for retrieving key PACE ocean geophysical parameters. In each subsection, we explain the justification for each requirement and identify additional desirables beyond the minimum requirements that could enhance the scientific benefits of the PACE mission. At the end of each subsection, minimum requirements and beneficial capabilities are summarized. We emphasize that the beneficial attributes do not represent a trade-space for achieving minimum requirements, but instead represent an advantage only if accomplished *in addition* to meeting all PACE minimum requirements. Finally, and before beginning this discussion of measurement requirements, we reiterate that success of PACE science relies not only on the exceptional satellite measurement capabilities defined herein, but also on a comprehensive mission design that integrates a rigorous calibration/validation program, repeated data reprocessing, and field-based research for algorithm development and product validation. These broader mission requirements are discussed in detail in other sections of this SDT report.

Measurement Requirements

1) Orbit: It is recommended that a near-noon sun-synchronous polar PACE orbit be chosen because it (1) provides high illumination intensities for accurate retrievals from the relatively dark ocean, (2) minimizes atmospheric path lengths for improved atmospheric corrections, (3) minimizes the range of scattering angles for simplification of atmospheric corrections and surface bidirectional reflectance effects, (4) maximizes repeat observations of high latitudes to improve probabilities of viewing cloud-free scenes each day and (5) observe as much of the earth as rapidly as possible. Based on experience with heritage ocean color sensors, a noon equatorial crossing time is optimal for addressing these considerations, although a window of 11:00 to 1:00 could be considered if a non-noon orbit within this wider window provides significant advantage for other science communities served by the PACE ocean radiometer (note, for a morning crossing time, a descending orbit is recommended; for an afternoon crossing time, an ascending orbit is recommended). In addition, it is recommended that the PACE orbit be maintained over the mission lifetime to ± 10 minutes to ensure that the heating and cooling cycles of the

spacecraft remain constant, which reduces potential sensor characterization issues. The preferred orbit altitude for PACE is ~700 km to provide the ~-day coverage.

Minimum Requirement: Sun-synchronous, polar orbit with an equatorial crossing time between 11:00 and 1:00, with orbit maintained to ± 10 minutes over the lifetime of the mission.

Beneficial: Sun-synchronous, polar orbit with noon equatorial crossing time and altitude of ~700 km.

2) Spatial and Temporal Coverage: The PACE ocean radiometer will provide observational data for applications across a wide range of space and time scales. Within the temporal domain, issues include maximizing successful matchups between field and satellite observations, tracking of bloom dynamics, and achieving clear-scene observations within a given period in a cloud-dominated atmosphere. Based on experience with heritage ocean color sensors, global observations every two days yield an adequate global fraction of clear-sky scenes to allow global-scale ecological and biogeochemical computations at 8-day resolution. For more regional analyses, 2-day global coverage can allow evaluations at 1-4 day resolution (note that 2-day global coverage typically means that many regions of the ocean are viewed at least once per day). A polar orbit with two-day global coverage also ensures that multiple views per day are achieved at higher latitudes, thus improving the probability of clear-sky scenes in these particularly cloudy regions. It is therefore recommended that 2-day global coverage is the minimum requirement for PACE within a solar zenith angle of 75° . However, 1-day global coverage is viewed as advantageous for improving the temporal resolution of science investigations if contemporary technologies allow this advance without compromising other measurement requirements for PACE. To achieve PACE global coverage requirements, view zenith angles relative to surface normal should not exceed 60° , as broader angles result in long atmospheric pathlengths (increased uncertainty in atmospheric correction) and can be associated with large pixel expansion (depending on instrument design). In addition, an important 'lesson learned' from heritage instruments is that avoidance of sun glint is critical for maximizing successful retrieval coverage for a given instrument design and for maximizing matchup observations with field calibration/ validation data. Thus, sun glint avoidance is an integral component of the minimum global coverage requirement for the PACE ocean radiometer. Glint avoidance was achieved with the SeaWiFS sensor using a $\pm 20^\circ$ tilt mechanism and a similar approach for PACE can be considered a low-risk option, although alternative approaches may be considered if they can achieve equivalent glint avoidance.

Minimum Requirement: 2-day global coverage to solar zenith angle of 75° , sun glint avoidance, multiple daily observations at high latitudes, and sensor view zenith angles not exceeding 60° .

Beneficial: 1-day global coverage. Coverage to $>75^\circ$ solar zenith angle.

New section – navigation & registration requirements (Fred Patt others?)

- Pointing knowledge
- Smear
- Jitter

- Co-registration
- Simultaneity

3) Instrument Performance Tracking: A key component of multiple PACE Ocean Science questions is the detection of temporal changes in ocean ecological and biogeochemical properties and processes. Many of these phenomena exhibit strong variability on diel to seasonal time scales. However, a fundamental motivation for the PACE mission is its contribution to the ocean climate data record and advancement of understanding regarding climate-ecosystem relationships. Importantly, the magnitude of inter-annual changes, or ‘anomalies’, in ocean ecosystem properties is often much smaller than their shorter time-scale variability. Consequently, characterizing inter-annual anomalies demands an accurate knowledge of temporal changes in instrument performance. Thus, a requirement for PACE is that degradation/drift in instrument performance be tracked at minimum on a monthly basis through observations of a stable external source (e.g., moon). These observations will be made through the instrument Earth-viewing port and using the same optical path as employed for ocean observations, as this approach minimizes uncertainties in performance characterization associated with changes in components that are not involved in the geophysical retrievals. Changes in instrument radiometric performance should be characterized on orbit for primary science measurement bands to a minimum requirement of $\pm 0.2\%$ and goal of $\pm 0.1\%$ within the first 3 years of the mission and maintained thereafter at this accuracy or better for the duration of the mission. Based on experience with heritage ocean color sensors, this minimum requirement has been achieved by SeaWiFS through monthly lunar observations at a constant phase angle, where all detectors are illuminated during each lunar maneuver. Employing an equivalent approach for the PACE ocean radiometer for performance tracking can thus be viewed as a low-risk option. Alternative approaches could also be considered if their effectiveness is clearly demonstrated prior to instrument selection for the PACE mission. Experience with heritage sensors indicates that tracking of performance changes in instruments with large detector arrays (e.g., MERIS, OCM-2) has been challenging because (1) only a fraction of the detectors are illuminated during a given lunar maneuver and (2) characterization using solar measurements has the added uncertainty of solar diffuser degradation trending. It should also be noted that instruments like MODIS suffer from a scan angle dependent degradation, which adds complexity to the calibration process because the calibration sources (moon and solar diffuser) are only available at selected scan angles (i.e., the degradation measurements must be extrapolated to the remaining scan angles, which – particularly for blue wavelengths – has led to a significant decrease in calibration accuracy. It is essential that these experiences with heritage sensors be carefully considered when evaluating whether a given approach for PACE measurements will enable success in the mission’s key objective of achieving sustained, climate-quality global ocean products.

An additional requirement for instrument performance tracking is daily measurements of a calibration target to allow detection of sub-monthly changes in instrument performance. For SeaWiFS, instrument performance changes were a remarkably smooth function of time and adequately characterized by monthly lunar observations. However, daily measurements of a calibration target and dark currents are recommended for PACE to ensure that any unforeseen step-changes in performance can be identified and accounted for. It is recommended that the additional calibration measurements be conducted by viewing an external source (e.g., solar

views using diffusers -as with heritage sensors), rather than an on-board light source. Temporal degradation of this daily calibration source should be known to $\sim 0.2\%$ between lunar observations. Finally, the PACE requirement for high spectral resolution measurements (see below) results in a minimum requirement for a capability to characterize instrument spectral drift over the mission lifetime. A variety of specific approaches may be considered for achieving this requirement, but spectral drift should be detectable and correctable to a minimum accuracy of ~ 0.3 nm.

Minimum Requirement: Monthly characterization of change in all instrument detectors and Earth-viewing optical components through measurement of a stable illuminated source (e.g., moon) through the Earth viewing port. Characterization of instrument radiometric performance changes to $\pm 0.2\%$ within the first 3 years of the mission and maintenance of this accuracy thereafter for the duration of the mission. Monthly characterization of instrument spectral drift to an accuracy of 0.3 nm. Daily observations of a calibration target/source (e.g., sun) and dark current for high temporal resolution tracking.

Beneficial: Characterization of instrument performance changes to $\pm 0.1\%$ within 3 years and maintenance of this accuracy thereafter.

4) Instrument Artifacts: The PACE mission aims to address current issues in global ocean ecology and biogeochemistry through the climate-quality retrieval of a broad suite of key ocean properties and processes. Success in this endeavor relies on accurate retrievals of spectral normalized water leaving radiances (nL_w). It is desired for PACE that uncertainties in nL_w be largely defined by state-of-the-science atmospheric correction errors, with contributions from uncharacterized instrument artifacts kept to an absolute minimum. These instrument artifacts contribute directly to radiance retrieval uncertainties and thus to errors in derived geophysical parameters. Instrument issues of concern include (but are not limited to) uncharacterized temporal changes in detector performance that give rise to image striping, optical or electronic crosstalk, polarization sensitivity, detector saturation, and scan-angle-dependent responses. Minimum requirements regarding these specific issues are defined below. More broadly, a minimum requirement is that the PACE instrument be thoroughly characterized pre-launch and that a post-launch approach be defined for tracking changes [see (3) above]. Pre-launch characterization should address all of the instrument properties described in *Section 3* of Meister et al. (2011), such as dynamic range, linearity, polarization and temperature sensitivity, saturation and recovery, out-of-band responses, stability, and response-versus-scan angle, to name a few. Effective pre- and post-launch characterization is essential for retrieving accurate TOA radiances during Level 0 to Level 1 processing, and is the foundation for achieving climate-quality Level 2 geophysical properties. Uncertainties in nL_w associated with uncharacterized instrument artifacts place a greater demand on atmospheric correction accuracies to meet minimum requirements for nL_w retrievals (see below). For PACE, these nL_w requirements are already near the ceiling of demonstrated atmospheric correction accuracies. Experience with heritage sensors indicates that instrument artifacts can be reduced to $< 0.5\%$ of top-of-atmosphere (TOA) radiances given an effective approach for characterizing the performance and degradation of all detectors (i.e., SeaWiFS), although this success has not been realized for most heritage instruments. The requirement for PACE is that the total error budget for a given observation be $\sim 0.5\%$ or less (this needs to be revisited)

Image Striping

Uncharacterized differences in the responsivity of multiple detector elements larger than the sensor noise (NedL) within a common spectral band results in an instrument artifact referred to as ‘image striping’, and susceptibility to this problem is linked to instrument design and ability to uniformly illuminate all detectors during on-orbit calibration maneuvers [see section (3) above]. The only ocean color sensor that achieved Level 2 products without notable image striping was SeaWiFS. All other heritage sensors (national and international) have yielded geophysical properties with significant cross-track and/or along-track striping. For PACE, the recommended minimum requirement is that corrected products exhibit no image striping at sensor measured spectral radiance (i.e., striping is less than sensor noise). A defining metric of PACE data product quality will be the performance of satellite retrievals against coincident field-based measurements. These validation data sets are compared at the pixel level and therefore performance metrics are directly degraded by instrument image striping. Similarly, satellite-field data comparisons for post-launch instrument calibration/gain setting are conducted at the pixel level and are thus also negatively impacted by striping, with a consequence (at best) of increasing the number of match-up data necessary for calibration and thus delaying achievement of climate quality data products.

Optical and Electronic Crosstalk

Crosstalk is defined as an erroneously measured signal for a given measurement wavelength and pixel spatial coordinate that originates from (spatial or spectral) stray light and/or the interaction of electro-magnetic fields between neighboring circuits. Crosstalk effects are very difficult and time consuming to quantify and require complicated algorithms to correct. Optical and electronic crosstalk issues have been a particular concern for VIIRS because of problems with optical filter strips and the compactness of the focal plane electronics, but issues were also experienced with SeaWiFS and MODIS. The recommended minimum requirement for crosstalk contributions to radiance uncertainties for PACE is 0.1% at L_{typ} .

Stray light and bright target recovery

Gerhard

Out of band response

Bryan and Gerhard

Polarization Sensitivity

The response of an ocean color instrument to completely linearly polarized light is expected to vary as a function of the polarization phase angle (which describes the axis of vibration of the electric field vector; Meister et al., 2005). Gordon et al. (1998) indicate that a 2% polarization sensitivity can lead to errors in the atmospheric correction that increase the uncertainty of the resulting nLw at 443nm by up to 10%. Given this sensitivity, the recommended upper limit for

the polarization sensitivity for PACE is 1%. The SeaWiFS design minimized inherent polarization sensitivity by limiting the angle of incidence range for light on its half-angle mirror (HAM), whereas the MODIS rotating mirror had a much larger range and the area of reflection off the mirror into the aft optics varied across the mirror during the scan (which is why the mirror had to be so large) (Meister et al. 2011). SeaWiFS also employed a depolarizer. For PACE, the recommended minimum requirement is knowledge of polarization sensitivity to an accuracy within 0.2% (most of the TOA radiances have a degree of linear polarization of less than 50%). A knowledge accuracy of 0.2% leads to an uncertainty in TOA radiances due to polarization of less than 0.1% for a large majority of global ocean cases (Meister et al. 2011). This polarization requirement for PACE is consistent with recommendations from the ACE science team [see Appendix of ACE Ocean Biology White paper (2010)].

Detector Saturation

Detector saturation is a potential issue for ocean color remote sensing because the signal from clouds and the atmosphere is very high compared to that from the ocean. When saturation occurs, it becomes extremely difficult to correct sensor data for stray light and, for instruments employing CCD arrays, saturation results in blooming of electrons in the detector spatial and spectral dimension. Furthermore, a finite detector recovery time is required following saturation (hysteresis), during which ocean color retrievals are invalid. Finally, the PACE ocean radiometer is intended to serve the scientific objectives of both the oceanographic and atmospheric communities. Thus, accurate radiance retrievals are required during bright scenes (i.e., clouds, aerosols) for many PACE measurement bands, which cannot be achieved with saturated detectors. Taken together, these considerations lead to the recommended minimum requirement for PACE that no saturation should occur for any science measurement bands at L_{\max} . Given this minimum requirement, it should also be noted that for a small number of instances, TOA radiances can exceed L_{\max} by up to $1.2 \times L_{\max}$ (Meister et al. 2011). It may therefore be viewed as beneficial if saturation is still avoided by the selected PACE instrument under these rare occasions. (need some text here that addresses linearity and its characterization – perhaps ‘beneficial’ to track on orbit – minimum requirement is well characterized prelaunch)

Response versus View Angle

In scanning ocean color sensors, significant variations in photon collection efficiency can occur as a function of scan angle. This ‘response versus scan angle’ (RVSA) issue was not a significant problem for the SeaWiFS because of its rotating telescope design, but it has been a major issue for the large rotating mirror of MODIS. While a significant RVSA dependence was recognized early-on for MODIS and characterized prelaunch, the daunting challenge for MODIS data processing has been that the RVSA has been changing over time, with few on-orbit options for characterizing these variations. The MODIS problem was worsened by mirror-side differences in performance properties. Given the primary objective of the PACE ocean radiometer of achieving a climate quality ocean color data set, it is essential that RVSA artifacts be minimized to the greatest extent possible. It is therefore recommended as a minimum requirement that the response of the PACE radiometer to a constant radiance source varies with view angle by <5% for the entire scan angle range and by <0.5% for scan angles that differ by less than 1° . The RVSA properties of the PACE radiometer should be characterized pre-launch

to an accuracy of 0.1% over the TOA radiance range corresponding to valid ocean color retrievals (this range is wavelength dependent and, based on SeaWiFS data, is 50 to 125 $W (m^2 \mu m sr)^{-1}$ at 412 nm and 2.2 to 16 $W (m^2 \mu m sr)^{-1}$ at 865 nm (Table 3.2 in Meister et al 2011)). (replace all ‘scan’ with ‘view’ and change RVSA to RVVA)

Minimum Requirement: Thorough prelaunch instrument characterization of linearity, RVSA, polarization sensitivity, radiometric and spectral temperature sensitivity, high contrast resolution, saturation, saturation recovery, crosstalk, radiometric and band-to-band stability, bidirectional reflectance distribution, and relative spectral response (see Meister et al. 2011 for details). Post-launch approach for tracking performance changes [see (3) above]. Overall instrument artifact contribution to TOA radiance retrievals of <0.5%. No image striping in Level 2 products and above. Maximum crosstalk contribution to radiance uncertainties of 0.1% at L_{typ} . Knowledge of polarization sensitivity to an accuracy $\leq 0.2\%$ and uncertainty in TOA radiances due to polarization of $\leq 0.1\%$. No detector saturation for any science measurement bands at L_{max} . RVSA of <5% for the entire scan angle range and by <0.5% for scan angles that differ by less than 1° .

Beneficial: Overall instrument artifact contribution to TOA radiance retrievals of <0.2%. No detector saturation for any science measurement bands up to $1.2 \times L_{max}$

5) Spatial Resolution: PACE ocean ecosystem and biogeochemical science questions require evaluations that span from globally-integrated climate-ecosystem relationships occurring over interannual time scales, to daily/weekly variability in spatially-heterogeneous near-shore waters, to single-point matchups with field samples for satellite product validation. Across all ocean domains observed and investigated by PACE, major advances in scientific understanding over heritage sensors will be realized through the improved separation of optically-active in-water constituents offered through PACE’s expanded spectral range and spectral resolution (see Ocean Ecosystem and Biogeochemistry Introduction section). Thus, the minimum requirement for spatial resolution for PACE is 1 km x 1 km along-track. For a scanning instrument with a maximum view zenith angle of 60° and altitude of 700 km (see above), this minimum spatial requirement yields a median pixel size of 1.4 km and average pixel size of 2.0 km across the scan. A PACE ocean radiometer that achieves 1 km x 1 km resolution across the entire scan may be viewed as advantageous, but only if this improved spatial resolution can be achieved without compromising other critical PACE measurement requirements (as defined herein). It is also advantageous for PACE to achieve higher spatial resolution in water masses near land, for either the entire PACE band set or for selected bands targeting key derived products. In these regions, spatial heterogeneity is generally greater than in the open ocean. For coastal, estuarine, and inland water systems, an along-track spatial resolution between 250 m x 250 m and 500 m x 500 m is beneficial, but achieving this resolution should not compromise other critical measurement requirements for 1 km global data (e.g., see different SNR requirements for higher spatial resolution data in section 8).

Minimum Requirement: Global coverage with a minimum spatial resolution of 1 km x 1 km along-track, becoming coarser across the scan to the maximum view zenith angle of 60° .

Beneficial: Global open-ocean spatial resolution of 1 km x 1 km at all scan angles and/or enhanced spatial resolution over inland, estuarine, coastal, and shelf areas of 250 m x 250 m to 500 m x 500 m for all bands or a subset of bands.

6) Atmospheric Corrections: A major challenge of passive ocean color remote sensing is that the atmosphere typically contributes >85% of the top-of-atmosphere radiance measured by the satellite sensor. This atmospheric signal must therefore be adequately removed to retrieve useful ocean ecosystem and biogeochemical parameters. Experience with heritage ocean color sensors indicates that scientifically useful global ocean products can be achieved over the open ocean under typical marine atmospheres using correction bands in the near infrared (NIR). It is therefore recommended, as a minimum requirement for PACE, that two measurement bands in the NIR be included that are comparable to heritage NIR bands in their value for atmospheric corrections and which preferably avoid major atmosphere absorption features (e.g., water vapor, O₂). Using these bands and including the additional sources of uncertainty described above, it is recommended that the minimum requirement for PACE normalized water leaving reflectance (nR_w) accuracies at visible wavelengths be the maximum of either 5% or 0.001 for open-ocean, clear-water conditions and under standard marine atmospheres (note that this minimum requirement is stated in terms of nR_w , rather than nL_w , to remove the wavelength dependence of the requirement). (Menghua & Jeromy will write a sentence here.) This accuracy requirement imparts an equal or smaller uncertainty on derived geophysical parameters (depending on the parameter retrieval algorithm - e.g., inversion or wavelength ratio) and will typically represent <15% of the total uncertainty associated with the derived ecosystem properties (i.e., the dominant uncertainty is associated with derivation of geophysical properties from nL_w and reducing this source of uncertainty requires algorithm development and field measurements). The science measurement spectral range for PACE also includes wavelengths in the near-ultraviolet (NUV: 350-400 nm). For these wavelengths which are more distal to the NIR bands, atmospheric corrections can be complicated by the presence of uncharacterized absorbing aerosols. However, spectral features of absorbing components in the NUV are strong, which somewhat reduces the accuracy requirement for nR_w at these wavelengths. It is therefore recommended that the minimum requirement for PACE nR_w accuracies in the NUV be the maximum of either 10% or 0.002 for open-ocean, clear-water (e.g., chlorophyll concentrations < 0.1 mg m⁻³) conditions and under standard marine atmospheres.

Minimum nR_w accuracy requirements defined above are for atmosphere and ocean conditions representative of broad regions of the global open ocean that are central to the science aims of PACE. However, additional conditions exist over important ocean regions where atmospheric corrections are more challenging. As noted above, one such challenging condition is retrieval of accurate nR_w under atmospheres with significant absorbing aerosols. These conditions are common near urban areas and under the dominant transport trajectories of desert dust sources (which can extend over broad open-ocean areas). Based on experience with heritage ocean color sensors, it should be expected that accurate ocean retrievals will generally not be achieved where aerosol optical thicknesses (AOT) exceed 0.3. At AOT < 0.3, successful retrievals are more likely, but absorbing aerosols can still be problematic, especially in the NUV and at short visible wavelengths. It is therefore recommended that the PACE ocean radiometer include a measurement band centered at 350 nm to either aid in the retrieval of ocean properties in the presence of absorbing aerosols through constraint of the atmospheric correction NIR-to-NUV

spectral slope, or to at least flag these potentially problematic aerosol-impacted pixels. Furthermore, additional aerosol data from a coincident sensor (e.g., multi-angle, multi-wavelength polarimeter on PACE or other platform), ground-based measurements (e.g., AERONET, aerosol transport models, etc.), and/or atmospheric models would be advantageous for integration into the atmospheric correction models for the PACE ocean radiometer data. This additional information will be particularly beneficial if it also includes information on aerosol heights (see also discussion in the atmospheric section of this document regarding a PACE radiometer O₂ band for height information). (Robert – few sentences here regarding polarimeter) In the absence of such ancillary aerosol data, it can be anticipated that uncertainties in nR_w will be somewhat larger when absorbing aerosols are present than the minimum required accuracies stated above for the case of standard marine atmospheres. Another complication for atmospheric corrections near urban pollution sources is the presence of nitrous oxide (NO₂). This issue has been evaluated for heritage sensors using ancillary NO₂ data measurement sources. Spatially and temporally varying ozone concentrations also impact the accuracy of ocean color atmospheric corrections. It is therefore recognized as advantageous for PACE ocean retrievals that measurement bands be included or ancillary data sets identified for NO₂ and ozone concentrations.

As described in the Ocean Ecosystem and Biogeochemistry introduction, the standard atmospheric correction approach applied to open ocean conditions can be problematic for turbid, near-shore areas because NIR water leaving reflectances in these waters are significant. This issue can be addressed using measurements in the shortwave infrared (SWIR). Based on experience with heritage sensors, SWIR bands in the spectral region of 1240 to 2130 nm are adequate for this application. It is therefore recommended as a PACE goal, 2- 3 measurement bands in the SWIR be included for atmospheric corrections over turbid waters and which avoid major atmosphere absorption features.

Minimum Requirement: Retrieval of normalized nR_w for open-ocean, clear-water conditions and standard marine atmospheres with an accuracy of the maximum of either 5% or 0.001 over the wavelength range 400 – 700 nm. Inclusion of NIR and SWIR bands for atmospheric correction that avoid major atmosphere absorption features. Inclusion of a NUV measurement band centered near 350 nm for flagging absorbing aerosols or improving atmospheric corrections through spectral anchoring.

Beneficial: Measurement of aerosol vertical distributions and type for improved atmospheric correction of PACE ocean radiometer data. Identification of ancillary data sets or PACE measurements of NO₂ and ozone concentrations at sufficient accuracy for improving atmospheric corrections.

7) Science Spectral Bands: In the Ocean Ecosystems and Biogeochemistry Introduction (OEBI), each overarching Science Question is associated with a specific set of geophysical properties or processes, although multiple overlaps in retrieval requirements exist between questions. The suite of required property/process retrievals can be grouped into ‘*primary level parameters*’ that are most closely related to the retrieved spectral nLw, ‘*secondary level parameters*’ that are derived from the primary parameters using ancillary field/satellite data and/or model input, and ‘*tertiary properties/processes*’ that are largely model-derived but

informed by the primary and/or secondary products. The 16 *primary level parameters* identified in the OEBI are subdivided below into four basic categories, with baseline and threshold retrieval ranges for each defined in Appendix I:

- Inherent optical properties (IOPs): total absorption coefficient (a), phytoplankton pigment absorption coefficient (a_{ph}), colored dissolved organic material absorption coefficient (a_{CDOM}), spectral slope of a_{CDOM} , particulate backscatter coefficient (b_{bp}), spectral slope of particulate backscatter coefficient,
- Apparent optical properties (AOPs): Spectral diffuse attenuation coefficient ($K_{d(\lambda)}$), Euphotic depth (Z_{eu}),
- Phytoplankton characteristics: biomass (C_{phyto}), chlorophyll (Chl), taxonomic/functional groups [including calcifiers, nitrogen fixers, carbon exporters (e.g., diatoms), harmful algal blooms], chlorophyll fluorescence, and
- Particle population characteristics: total suspended particulate matter, particulate organic carbon concentration, particulate inorganic carbon concentration, dominant particle size classes or mean particle size

Together with atmospheric correction requirements discussed above, retrieval of these 16 parameters drives the ocean requirements for PACE spectral range and spectral resolution.

Links between specific spectral regions and retrieval objectives are detailed in the OEBI and yield a recommended minimum ocean requirement for spectral range (excluding atmospheric correction bands – see above) of 355 to 800 nm. Within this range, the minimum requirement for spectral resolution is 5 nm, as defined by the coarsest resolution necessary for phytoplankton taxonomic discrimination using spectral derivative analysis techniques. Finer spectral resolution is advantageous for derivative analyses, but is only desirable if it does not compromise other critical minimum requirements. A primary purpose of taxonomic retrievals using derivative analyses is to improve understanding of phytoplankton community composition and succession in the open ocean, and major advances can be made to this end with 5 nm resolution PACE data even if a somewhat reduced spatial resolution is necessary to achieve adequate signal-to-noise ratios [see subsection (8) below]. In addition to taxonomic analyses, the 5 nm NUV-through-visible requirement is desired to allow reconstruction of heritage ocean color bands and for flexibility in assembling aggregate bands for new science applications. Accordingly, downlink of the complete 5 nm resolution (or finer) data from the spacecraft to (a) ground station(s) and archival of these data is a minimum requirement for PACE.

Aside from retrieval of phytoplankton taxonomic information, 5 nm resolution bands are not necessary for the other *primary level parameters*, as these parameters are derived from coarser spectral features. For these applications, retrievals can employ spectral bands of order ~15 nm breadth that are created by aggregating 5 nm resolution data. This aggregation provides improved signal-to-noise ratios (relative to 5 nm resolution data) for a given spatial resolution. It should be noted that allowable spectral aggregation for the chlorophyll fluorescence is narrower than that for most other primary products. Based on experience with heritage sensors, characterization of the chlorophyll fluorescence feature requires a maximum bandwidth of ~10 nm centered around 680 nm. This narrower band is constrained on the short wavelength side by the distribution of the chlorophyll emission spectrum and on the long wavelength side by a

strong atmospheric oxygen absorption feature. Furthermore, it would be advantageous for PACE to have a capacity for finer spectral resolution between 665 and 700 nm to more accurately characterize the fluorescence emission band and assess fluorescence quantum yields. Finally, the primary science objective for the PACE fluorescence product is the characterization of open-ocean nutrient stressors, particularly iron (note that fluorescence products in optically complex coastal zones are contaminated by particle scattering contributions). For this application, a spatial resolution in fluorescence line height products of 2 km x 2 km is acceptable for improving signal-to-noise ratios for this challenging ocean property retrieval.

Secondary level parameters identified in the OEBI include dissolved organic carbon concentration (DOC), photobiochemical transformations, phytoplankton physiological properties, and net primary production (NPP). DOC is included in this parameter category because no clear relationship has yet been identified to globally relate DOC to any *primary level parameter*. However, DOC has been estimated from a_{CDOM} for some near-shore regions using ancillary field data. One of the important carbon-relevant photobiochemical transformations is the degradation of CDOM. For PACE, aggregate spectral bands in the NUV and short visible wavelengths will allow retrieval of a_{CDOM} and the spectral slope of a_{CDOM} . Combining these *primary level parameters* with ancillary data on incident UV flux and photodegradation efficiencies will allow global assessments of CDOM degradation. The OEBI also identifies phytoplankton physiological properties as essential PACE products because information on physiological status allows evaluation of changing nutrient and light stress conditions and is essential for assessment of NPP. Key physiological properties retrievable from PACE *primary level parameters* are fluorescence quantum yield (ϕ), chl:C_{phyto}, and a_{ph} :C_{phyto}. Finally, a diversity of algorithms has been developed for assessing NPP, with each approach requiring multiple *primary level parameters* (e.g., Chl, C_{phyto}, a_{ph} , $K_{d(*)}$, Z_{eu} , etc.) and other ancillary properties (e.g., photosynthetically active radiation, SST, MLD, etc.).

Key *tertiary properties/processes* include the ocean surface export carbon flux, net community production, air-sea CO₂ exchange, land-ocean material exchange flux, and ocean radiant heating and its biological feedbacks. As described in the OEBI, assessment of these global properties/processes is an important science goal for PACE that is reliant on an integrated modeling component to the mission, where the *primary and secondary level parameters* described above contribute to model development/refinement by providing observational constraints on key ocean properties.

Minimum Requirement: 5 nm spectral resolution from 350 to 750 nm, in addition to spectral bands identified in section 6 for atmospheric corrections. Complete ground station download and archival of 5 nm data.

Beneficial: Spectral subsampling at ~1-2 nm resolution from 655 to 700 nm for refined characterization of the chlorophyll fluorescence spectrum, in addition to spectral subsampling identified in section 6 for NO₂ detection.

8) Signal-to-noise: Achieving climate-quality ocean data products is a foremost objective of the PACE mission. In the subsections above, we have recommended (in addition to other attributes) spatial and spectral minimum requirements necessary to realize central science objectives of the

PACE mission, as well as desirable improvements beyond these minimum requirements for further science benefits. In addition to these specifications, it is essential that minimum requirements be defined regarding signal-to-noise ratios (SNR), as instrument noise contributes to uncertainties in derived parameters. To evaluate SNR requirements, model studies were conducted that quantified retrieved parameter uncertainties associated with instrument noise in the atmospheric correction bands and NUV-visible (science) bands (see Appendix I). For this analysis, two NIR (765 and 865 nm) and three SWIR (1240, 1640, and 2130 nm) atmospheric correction bands were included, along with NUV through visible science bands spaced 10 to 15 nm apart (10 nm spacing for fluorescence bands only).

For both atmospheric corrections and ocean science parameters, retrieval errors decrease exponentially toward an asymptote as SNR increases (Appendix I). Minimum SNR requirements for PACE were taken as those values where the mean error becomes stable (i.e., approaches the asymptote). The resultant recommended SNR requirements are summarized in Table 1 for NUV and visible band centers spaced 15 nm apart and for representative NIR and SWIR bands for atmospheric applications. The uniform SNR requirements shown in Table 1 for most NUV-visible bands imply that precise band centers are not critical to the SNR analysis results. It

λ	L_{typ}	L_{max}	SNR-spec
350	7.46	35.6	300
360	7.22	37.6	1000
385	6.11	38.1	1000
412	7.86	60.2	1000
425	6.95	58.5	1000
443	7.02	66.4	1000
460	6.83	72.4	1000
475	6.19	72.2	1000
490	5.31	68.6	1000
510	4.58	66.3	1000
532	3.92	65.1	1000
555	3.39	64.3	1000
583	2.81	62.4	1000
617	2.19	58.2	1000
640	1.90	56.4	1000
655	1.67	53.5	1000
665	1.60	53.6	1000
678	1.45	51.9	1000
710	1.19	48.9	1000
748	0.93	44.7	600
765	0.83	43.0	600
820	0.59	39.3	600
865	0.45	33.3	600
1245	0.088	15.8	250
1640	0.029	8.2	180
2135	0.008	2.2	100

should also be noted that a PACE instrument that achieves SNRs greater than these minimum requirements offers some advantage, as a modest decrease in retrieval errors results from higher SNRs.

Table 1. PACE SNR minimum requirements. For wavelengths between 360 and 655 nm, a representative set of bands are shown, but additional or different band centers may be appropriate as defined herein by PACE science spectral requirements. λ = wavelength of band center. **L_{typ}** = typical top-of-atmosphere clear sky ocean radiances. **L_{max}** = saturation radiances. **SNR spec** = minimum SNR requirement at L_{typ}. Radiance units are mW/(cm² μm sr).

An important aspect of our SNR requirements evaluation is that the chosen criterion for selection is an SNR where the mean error becomes stable. Specifications in Table 1, therefore, provide a spectral distribution of SNR requirements for climate quality ocean product retrievals that is independent of spectral band width and spatial resolution. As stated in subsection (7) above, 14 of the 16 *primary level parameters* for PACE ocean science can be retrieved with spectral bandwidths in the NUV and visible of ~15 nm. Thus, for these global ocean products, SNR requirements (Table 1) at 1 km x 1km resolution (along-track) can be met by aggregating higher resolution data to 15 nm bins. For the NIR and SWIR atmospheric correction bands, SNR requirements (Table 1) can be met using bandwidths substantially broader than 15 nm (as with heritage sensors), so long as these broader bands avoid major atmospheric

absorption features. With respect to taxonomic discriminations using derivative analyses, SNR requirements in the visible wavelengths are still ≥ 1000 (Table 1), but at 5 nm resolution. These requirements, however, can be met by spatially aggregating data to, say, a 2 km or 4 km along-track resolution (as discussed above). Similarly, chlorophyll fluorescence products can be aggregated to 2 km along-track resolution to achieve adequate SNR. In subsection 4 above, we also stated that spatial resolutions finer than 1 km x 1 km are advantageous for near-shore studies. It is recognized that at this higher spatial resolution the resultant SNR will be lower than those defined in Table 1. It is recommended that potential PACE instruments define the SNR values that can be expected at these higher spatial resolutions.

Minimum Requirement: Instrument SNR at L_{typ} as defined in Table 1 for atmospheric bands, fluorescence bands, and NUV-visible bands at 15 nm resolution at all spatial resolution to which these bands are applied for PACE science. For 5 nm resolution data between 360 and 655 nm, an SNR of ≥ 1000 is required but at a spatial resolution of ≤ 4 km x 4 km. SNR may be relaxed at spatial resolution < 1 km x 1 km.

Beneficial: SNR greater than those shown in Table 1.

9) Data Processing, Reprocessing, and Distribution: The importance of reprocessing mission data at regular intervals throughout the mission became apparent during both SeaWiFS and MODIS missions (McClain, 2009; Siegel and Franz, 2010). Much is learned during a mission about a sensor's behavior and the atmospheric correction, bio-optical, and data high-quality mask/flag algorithms for converting L_w into ocean color products. Data reprocessing is needed to adjust for the following changes: (1) calibration coefficients due to sensor degradation, (2) in-water and atmospheric correction algorithms resulting from validation results, and (3) availability of new algorithms for improved data products. In addition, it takes many match-ups before a vicarious calibration can achieve the desired accuracy and stability for the sensor's gain factor. Therefore, data processing and product generation cannot be expected to produce high-quality products at the beginning of a mission. For all these reasons, data product quality will improve as more is learned about a sensor's behavior and as a result of reprocessing. For example, the initial processing of SeaWiFS imagery yielded negative values for water-leaving radiance for continental shelf waters in the band centered at 412 nm and depressed values at 443 nm. This difficult problem was not fully resolved until the data were reprocessed many times (e.g., Patt et al., 2003; McClain, 2009). In 2009, the reprocessing of the MODIS-Aqua dataset corrected another, much more subtle drift in the 412 nm water-leaving radiance band, which had resulted in an apparent dramatic increase in CDOM concentration in the open ocean (Maritorena et al., 2010).

Reprocessing of ocean color datasets also is critical for developing decadal-scale records across multiple missions. Antoine et al. (2005) developed a decadal-scale ocean color data record by linking the CZCS data record to the SeaWiFS era. Key to their approach was the reprocessing of both datasets using similar algorithms and sources. The resulting decadal ocean color time-series shows many interesting climate patterns supporting their approach (Martinez et al., 2009). Thus it is likely that the best approach to creating multi-decadal ocean color data products is the simultaneous reprocessing of multiple ocean color missions with similar algorithms and the same vicarious calibration sources, if possible (Siegel and Franz, 2010). Based on experience with

heritage data sets, it is strongly recommended that the PACE mission be designed, and resources (people, equipment, funding, etc) dedicated to, a capacity for full data reprocessing at a minimum frequency of 1 – 2 times annually. Furthermore, it is strongly recommended that the PACE mission establish a dedicated and consistent team for data processing, reprocessing, and distribution, as was employed during the SeaWiFS mission. (Dave volunteered to write some text here to address issues of data processing being different than in the past.)

Minimum Requirement: Capacity for full reprocessing of PACE data at a minimum frequency of 1 – 2 times annually.

Summary of PACE Ocean Science Measurement Requirements

In this section of the SDT report, we have defined specific minimum ocean science requirements for the PACE ocean radiometer and have identified additional capabilities that could extend the scientific contributions of the mission. These measurement requirements derive directly from the Science Objectives and Approaches detailed in the OEBI and reflect the mission's primary focus on achieving global ocean climate-quality data for extending the heritage ocean color record and addressing outstanding science issues inaccessible to the restricted capabilities of these earlier sensors. Throughout this section, we have identified specific approaches for meeting the measurement requirements based on experience with heritage sensors, but have also noted that alternative approaches should be considered if their effectiveness is clearly demonstrated. We have also emphasized that new approaches for meeting measurement requirements and/or for achieving the additional capabilities enabling expanded science contribution should only be considered if they do not compromise essential minimum measurement requirements for the mission. To aid NASA in this evaluation, we summarize in Table 2 (next page) the minimum requirements deemed essential for PACE threshold science objectives, followed by additional desirable capabilities that are not viewed as exchangeable with the essential minimal requirements.

Minimum Requirements

Beneficial

Orbit	<p>(1) Sun-synchronous polar orbit; (2) equatorial crossing time between 10:30 and 1:30; (3) orbit maintenance to ± 10 minutes over mission lifetime</p>	<p>(1) Sun-synchronous, polar orbit with noon equatorial crossing time</p>
Global Coverage	<p>(1) 2-day global coverage; (2) sunglint avoidance; (3) multiple daily observations at high latitudes; (4) swath width not exceeding $\pm 58^\circ$.</p>	<p>(1) 1-day global coverage.</p>
Instrument Performance Tracking	<p>(1) characterization of all detectors and optical components through monthly observations through Earth-viewing port of stable, external illuminated source (e.g., moon); (2) characterization of instrument performance changes to $\pm 0.2\%$ within the first 3 years and maintenance of this accuracy thereafter for the duration of the mission; (3) monthly characterization of instrument spectral drift to an accuracy of 3 nm; (4) daily observations of a calibration target/source (e.g., sun)</p>	<p>(1) Characterization of instrument performance changes to $\pm 0.1\%$ within 3 years and maintenance of this accuracy thereafter (2) Daily characterization of instrument spectral drift to an accuracy of 1 nm.</p>
Instrument Artifacts	<p>(1) Prelaunch characterization of linearity, RVSA, polarization sensitivity, radiometric and spectral temperature sensitivity, high contrast resolution, saturation, saturation recovery, crosstalk, radiometric and band-to-band stability, bidirectional reflectance distribution, and relative spectral response ; (2) overall instrument artifact contribution radiance uncertainty of $< 0.5\%$; (3) no image striping in Level 2 products and above; (4) crosstalk contribution to radiance uncertainties $\leq 0.1\%$ at L_{yp}; (5) knowledge of polarization sensitivity to $\leq 0.2\%$ and uncertainty in TOA radiances of $\leq 0.1\%$; (6) no detector saturation for any science measurement bands at L_{max}; (7) RVSA of $< 5\%$ for the entire scan angle range and by $< 0.5\%$ for scan angles that differ by less than 1°.</p>	<p>(1) Overall instrument artifact contribution to TOA radiance retrievals of $< 0.2\%$. (2) No detector saturation for any science measurement bands up to $1.2 \times L_{max}$</p>
Spatial Coverage	<p>(1) Global spatial coverage of 1 km x 1 km at nadir</p>	<p>(1) 1 km x 1 km resolution at all angles (2) 250 m x 250 m to 500 m x 500 m for coastal/ shelf regions</p>
Atmospheric Corrections	<p>(1) retrieval of normalized nR_w for open-ocean, clear-water conditions and standard marine atmospheres with an accuracy of the maximum of either 5% or 0.001 over the wavelength range 400 – 700 nm; (2) NIR and SWIR atmospheric correction bands comparable to heritage; (3) NUV band centered near 350</p>	<p>(1) Measurement of aerosol vertical distributions and type (1) Measurement of NO_2 concentration</p>
Science Spectral Bands	<p>(1) 5 nm spectral resolution from 350 to 750 nm; (2) complete ground station download and archival of 5 nm data.</p>	<p>(1) Spectral subsampling at ~ 1-2 nm resolution from 655 to 700</p>
Signal-to-noise	<p>(1) SNR at L_{yp} as defined in Table 1 for all science bands at the spatial resolution to which these bands are applied for PACE science.</p>	<p>(1) SNR greater than those shown in Table 1.</p>
Data Processing, Reprocessing, Distribution	<p>(1) full reprocessing capability of all PACE data at a minimum frequency of 1 – 2 times annually.</p>	

Appendix I

This appendix has three sections: (1) baseline and threshold retrieval ranges for optical, biological, and biogeochemical parameters related to ocean science questions, (2) atmospheric correction sensitivity to noise, and (3) bio-optical algorithm retrieval sensitivity to noise. Parameter baseline and threshold range were assembled by the ACE ocean science team. The atmospheric correction analysis was conducted by Menghua Wang (NOAA/NESDIS) and Howard Gordon (U. of Miami). The bio-optical algorithm study was conducted by Stephane Maritorena (UC/Santa Barbara) using inputs from the Wang and Gordon study.

(1) Ocean Optical, Biological, and Biogeochemical Parameters

Associated with each PACE science question is a set of geophysical parameters that must be measured in order to address the question. Remote sensing retrievals for each of these parameters require an algorithm that transforms the basic water-leaving radiances or remote sensing reflectances into an estimated value of that parameter over a range of values. In the following 6 pages, the various desired geophysical parameters are shown in the left-most column. For each parameter, the second and third columns indicate baseline and threshold ranges for the parameter, respectively. Here, the ‘baseline’ range represents the full desired retrieval range for a given parameter and is the range of values between the 1% and 99% region for the parameter frequency distribution. The ‘threshold’ range is the required retrieval range for a given parameter and represents the 5% to 95% region of the frequency distribution. Baseline and threshold values for the geophysical parameters were based on analyses of both field and historical satellite measurements. Specific information regarding these analyses for each parameter is provided in the right-most column of comments. It should be noted that values for each parameter have been measured that exceed even the baseline range, but these values are found under extreme and rare conditions and were not viewed as critical retrieval requirements for a satellite mission focused on global ocean properties.

Geophysical Parameter	Baseline Range	Threshold Range	Comments
Remote sensing reflectance (Rrs)	Rrs(340) 0.0015 - 0.020 sr ⁻¹ Rrs(380) 0.0017 - 0.020 sr ⁻¹ Rrs(412) 0.0011 - 0.033 sr ⁻¹ Rrs(443) 0.0016 - 0.024 sr ⁻¹ Rrs(490) 0.0023 - 0.014 sr ⁻¹ Rrs(510) 0.0026 - 0.011 sr ⁻¹ Rrs(531) 0.0021 - 0.010 sr ⁻¹ Rrs(547) 0.0014 - 0.009 sr ⁻¹ Rrs(555) 0.0014 - 0.008 sr ⁻¹ Rrs(670) 0.0000 - 0.002 sr ⁻¹ Rrs(678) 0.0000 - 0.002 sr ⁻¹ Rrs(683) 0.0000 - 0.012 sr ⁻¹	Rrs(340) 0.0020 - 0.015 sr ⁻¹ Rrs(380) 0.0030 - 0.017 sr ⁻¹ Rrs(412) 0.0035 - 0.028 sr ⁻¹ Rrs(443) 0.0038 - 0.021 sr ⁻¹ Rrs(490) 0.0042 - 0.012 sr ⁻¹ Rrs(510) 0.0036 - 0.008 sr ⁻¹ Rrs(531) 0.0027 - 0.006 sr ⁻¹ Rrs(547) 0.0019 - 0.005 sr ⁻¹ Rrs(555) 0.0018 - 0.005 sr ⁻¹ Rrs(670) 0.0001 - 0.001 sr ⁻¹ Rrs(678) 0.0001 - 0.001 sr ⁻¹ Rrs(683) 0.0000 - 0.001 sr ⁻¹	Ranges in the 412-678 nm region are based on the SeaWiFS and MODIS-AQUA data. Ranges at 340, 380 and 683 nm are based on field measurements from a variety of oceanic and coastal stations (n > 1,000) extracted from the NASA SeaBASS archive.
Inherent optical properties <i>Absorption coefficients</i> - total absorption (a) - phytoplankton absorption (a _{ph}) - detrital absorption (a _d) - colored dissolved organic material absorption (a _{CDOM})	a(412) 0.020 - 2.0 m ⁻¹ a(443) 0.020 - 1.8 m ⁻¹ a(555) 0.065 - 1.5 m ⁻¹ a(676) 0.460 - 1.8 m ⁻¹ a _{ph} (443) 0.003 - 1.2 m ⁻¹ a _d (443) 0.0004 - 0.6 m ⁻¹ a _{CDOM} (443) 0.002 - 0.9 m ⁻¹	a(412) 0.03 - 0.8 m ⁻¹ a(443) 0.03 - 0.7 m ⁻¹ a(555) 0.08 - 0.6 m ⁻¹ a(676) 0.47 - 0.8 m ⁻¹ a _{ph} (443) 0.007 - 0.7 m ⁻¹ a _d (443) 0.001 - 0.3 m ⁻¹ a _{CDOM} (443) 0.003 - 0.5 m ⁻¹	For total a and c, 1% and 5% values were based on OSU data base (450 near surface data points), 95% values based on data from the Philippines (PHILEX, two cruises), and the 99% values based on coastal OASIS observations. The a _{ph} , a _d , and a _{CDOM} values are based on NOMAD data (Mannino et al 2008, Nelson et al 2010). BIOSOPE data from the ultra-oligotrophic South Pacific gyre were used in assessing lower limits of baseline ranges (Huot et al., 2008; Bricaud et al., 2010).
<i>Backscatter coefficient (bb)</i> <i>Beam attenuation (c)</i>	b _{bp} (443) 0.0003 - 0.1 m ⁻¹ c(412) 0.03 - 10.0 m ⁻¹ c(443) 0.03 - 10.0 m ⁻¹ c(555) 0.08 - 10.0 m ⁻¹	b _{bp} (443) 0.001 - 0.003 m ⁻¹ c(412) 0.1 - 0.5 m ⁻¹ c(443) 0.1 - 0.5 m ⁻¹ c(555) 0.1 - 0.5 m ⁻¹	bbp(443) values are based on the GSM (Maritorena et al. 2002) and QAA (Lee et al 2002) inversion models applied to MODIS L3 data,

	c(676) 0.47 - 10.4 m ⁻¹	c(676) 0.5 - 0.9 m ⁻¹	<p>in addition to a subset of field measurements available in SeaBASS. Coastal, sediment-dominated waters have values well beyond the stated maximum.</p> <p>a_{CDOM} values are based on field data which contain sampling bias in coastal regions. Recommended maxima based on satellite data and field measurements from high CDOM areas (coastal & river plumes) are 3 m⁻¹ for threshold and 10 m⁻¹ for baseline.</p>
Diffuse attenuation coefficient for downwelling plane irradiance at 490 nm [Kd(490)]	Kd(490) 0.02 - 4.0 m ⁻¹	Kd(490) 0.02 - 1.5 m ⁻¹	<p>Based on >6,100 in-water profiles, spanning the clearest waters (South Pacific gyre, Arctic ice zone) to very turbid and shallow riverine waters. Values are based on data in the near-surface extrapolation interval--they are not "bulk" values (Morel et al. 2007). Kd can also be derived for other wavelengths.</p>
Incident Photosynthetically Available Radiation (PAR) <i>Instantaneous</i> <i>24-hr flux</i>	<p>0 - 2,200 μmol quanta m⁻² s⁻¹</p> <p>0 - 60 mol quanta m⁻² d⁻¹</p>	<p>100 - 2,100 μmol quanta m⁻² s⁻¹</p> <p>10 - 55 mol quanta m⁻² d⁻¹</p>	<p>In some partly cloudy situations, the upper values for instantaneous PAR can be 10-15% higher due to reflection by the side of clouds.</p> <p>Ranges for 24 hr PAR data based on 2004 MODIS data corrected for cloudiness and available at: oceancolor.gsfc.nasa.gov/</p>
1% PAR depth (Z_{1%})	10 - 150 m	35 - 135 m	<p>Ranges are based on 2008 MODIS Rrs retrievals, with the 1%PAR depth calculated following Lee et al. (2007).</p>

<p>Particulate inorganic carbon concentration (PIC)</p>	<p>1.2 * 10⁻⁵ - 5.3 * 10⁻⁴ mol m⁻³</p>	<p>1.9 * 10⁻⁵ - 3.3 * 10⁻⁴ mol m⁻³</p>	<p>Values based on Atlantic Meridional Transect cruises (covering the oligotrophic gyres to eutrophic waters). N=481. Samples processed by first filtering seawater onto 0.4µm polycarbonate filters and subsequently rinsed with potassium tetraborate (pH8), to rinse away seawater calcium. PIC derived from particulate calcium measurement using inductively-coupled plasma optical emission spectroscopy. Samples corrected for seawater calcium by also measuring the sodium line with the ICP-OES. Statistics calculated on log transformed data.</p>
<p>Particulate Organic Carbon concentration (POC)</p>	<p>15 - 2,000 mg m⁻³</p>	<p>20 - 500 mg m⁻³</p>	<p>Values based on 804 field measurements from ultra-oligotrophic to turbid coastal environments. Minimum and maximum surface values of POC derived from both field and satellite data are about 10 mg m⁻³ and 10,000 mg m⁻³. In extreme cases values in excess of 10,000 mg m⁻³ have been observed</p>
<p>Dissolved Organic Carbon concentration (DOC)</p>	<p>35-800 µmol L⁻¹</p>	<p>40-500 µmol L⁻¹</p>	<p>Values based on field data. Surface DOC in the field ranges from 35 to 1,000 µmol L⁻¹. Typical river plume DOC is 650 µmol L⁻¹ for Arctic and tropical rivers, but DOC can exceed 1,000 µmol L⁻¹.</p>
<p>Suspended Particulate Matter concentration (SPM)</p>	<p>25 - 70,000 mg m⁻³</p>	<p>45 - 15,000 mg m⁻³</p>	<p>Values based on 271 field measurements from ultra-oligotrophic to turbid coastal</p>

				environments. For this data set, the minimum SPM = 22 mg m ⁻³ and the maximum ~140,000 mg m ⁻³ . In some aquatic environments higher values can be observed.
Particle size characteristics (size ranges indicated here)	0.05 - 2,000 μm	0.8 - 200 μm		Threshold values reflect current measurement capabilities for seawater samples using electronic counting/sizing (e.g., Coulter) and laser diffraction (e.g., LISST). Baseline values represent a desired, environmentally-relevant range requiring near-term instrument/technique development.
Total Chlorophyll-a concentration (TChl-a)	0.015 - 40 mg m ⁻³	0.030 - 25 mg m ⁻³		Values based on field and satellite (SeaWiFS) data. Field data are from SeaBASS and include HPLC and Turner fluorescence measurements.
Other phytoplankton pigments	To be defined	To be defined		
Phytoplankton Carbon concentration (C_{phyto})	0.15 - 800 mg m ⁻³	3.0 - 450 mg m ⁻³		Values based on satellite retrievals of b_{bp} converted to C_{phyto} following Westberry et al. (2008).
Normalized Fluorescence Line-height (FLH)	0.0001 - 0.025 mW cm ⁻² μm ⁻¹ sr ⁻¹	0.001 - 0.015 mW cm ⁻² μm ⁻¹ sr ⁻¹		Values based primarily on MODIS L3 data, but in situ data (NOMAD) were also used for evaluating maximum criteria
Fluorescence Quantum Yield (FQY)	0.0003 - 0.05 fluoresced photons (absorbed photons) ⁻¹	0.001 - 0.02 fluoresced photons (absorbed photons) ⁻¹		Values based on MODIS L3 data following Behrenfeld et al. (2009), which includes a correction for non-photochemical quenching that reduces FQY values at low-light

Net Primary Production (NPP)	55 - 8,500 mg m ⁻² d ⁻¹	90 - 4,500 mg m ⁻² d ⁻¹	Values based on field and satellite (SeaWiFS) data. Satellite data are from the VGPM (Behrenfeld & Falkowski 1997). Field data are from the OSU productivity website: www.science.oregonstate.edu/ocean/productivity/
Phytoplankton physiological properties <i>Chl:C</i> <i>Growth Rate</i>	0.0005 - 0.3 mg mg ⁻¹ 0.00 - 1.9 d ⁻¹	0.001 - 0.1 mg mg ⁻¹ 0.01 - 1.5 d ⁻¹	Growth rate values based on satellite Chl:C data, light attenuation, and mixing depth (Westberry et al. 2008).
Phytoplankton groups <i>Size-based groups expressed as a fraction of total algal chlorophyll</i>	microphytoplankton: 0 - 0.9 nanophytoplankton: 0 - 0.9 picophytoplankton: 0 - 1.0	microphytoplankton: 0 - 0.7 nanophytoplankton: 0.2 - 0.8 picophytoplankton: 0 - 0.8	Size-based groups from exclusively open-ocean field HPLC- pigment data (Uitz et al. 2006), with a baseline surface chlorophyll-a range of 0.03 - 5.8 mg m ⁻³ . Only data from the first optical depth are included. See Uitz et al. (2006) for details. Alternative approaches for defining phytoplankton groups are also under investigation.
<i>Trichodesmium concentration</i>	0 - 10,000 filaments L ⁻¹	0 - 5,000 filaments L ⁻¹	Values based on ~20 years of field data (largely epifluorescence microscopy of filtered seawater). When necessary, filaments L ⁻¹ was estimated assuming 200 filaments colony ⁻¹ (Carpenter, 1983). A large bloom can exceed 10 ⁶ filaments L ⁻¹ .
<i>Coccolith concentration</i>	293 - 814,930 detached coccoliths mL ⁻¹ 34 - 3,624 plated	760 - 314,000 detached coccoliths mL ⁻¹ 59 - 2,066 plated	Values based on field data from Atlantic Meridional Transect cruise 17 (n=412 samples) which included oligotrophic to temperate waters and a coccolithophore bloom

	coccolithophores per coccolith aggregates mL ⁻¹	coccolithophores per coccolith aggregates mL ⁻¹	Statistics calculated on log transformed data. Note, highest published concentrations of detached coccoliths in the field are ~500,000 mL ⁻¹ . The baseline upper range of 800,000 mL ⁻¹ (statistically defined here by the upper 99 th percentile of log-normal variance), thus, appears high. Plated coccolithophores are combined with coccolith aggregates because discrimination is difficult when using birefringence microscopy.
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(2) Simulations for the NIR and SWIR SNR requirements for atmospheric corrections

Atmospheric correction for ocean color product is extremely sensitive to sensor spectral band calibration errors, as well as to radiometric noise. This is due to the considerably low radiance from the ocean compared to the sensor-measured top-of-atmosphere (TOA) radiance. The sensor spectral band radiometric performance can be characterized by the signal to noise ratio (SNR). To understand the radiometric noise effects on the derived normalized water-leaving reflectance spectra, simulations of atmospheric correction, using the two near-infrared (NIR) bands (765 and 865 nm) and various combinations of the shortwave infrared (SWIR) bands (1240, 1640, and 2130 nm), have been carried out for several levels of sensor noise.

Noise Model. A Gaussian distribution (with mean value = 0) is used for the noise simulations. The standard deviation (STD) of the Gaussian distribution is the radiance noise level (i.e., related to the SNR values). The simulated reflectance noise is then added into the TOA reflectance at various NIR and SWIR bands that are used for making atmospheric correction. Eight noise levels are generated, corresponding to eight SNR values of 25, 50, 100, 200, 400, 600, 800, and 1000. It is noted that the reflectance noise is only added into the bands that are used for atmospheric correction (e.g., two NIR bands), and UV and visible bands are noise free in all simulations discussed in this subsection. The reflectance noises are spectrally incoherent.

Atmospheric Correction. Atmospheric correction simulations using two NIR bands (Gordon and Wang, 1994) and various SWIR bands (Wang, 2007) have been carried out including reflectance noise levels for the corresponding NIR and SWIR bands. Specifically, simulations were carried out for a typical Maritime aerosol model (M80) and a Tropospheric model (T80), where the T80 model is actually M80 model without the large size fraction, for aerosol optical thicknesses (at 865 nm) of 0.05, 0.1, 0.2, and 0.3. The M80 and T80 aerosol models were not used in the aerosol lookup tables for atmospheric correction (Gordon and Wang, 1994; Wang, 2007). Simulations were performed for a case with solar-zenith angle of 60°, sensor-zenith angle of 45°, and relative azimuth angle of 90°.

SNR Simulations. For each case, atmospheric correction for 5000 noise realizations with a given SNR value was carried out. For example, for a case with aerosol optical thickness (AOT) at 865 nm of 0.1, 5000 reflectance noise samples (with a given SNR value) were generated and added into the TOA NIR (765 and 865 nm) reflectance values. The NIR atmospheric correction (Gordon and Wang, 1994) was then performed 5000 times to generate the corresponding normalized water-leaving reflectance spectra error. The same procedure was carried out for all four AOTs and also for the SWIR algorithm (Wang, 2007). In the SWIR atmospheric correction, however, the Gaussian noise was of course added into the SWIR bands (error free for UV to NIR bands). This produces the uncertainty in the derived normalized water-leaving reflectance from the UV to the red (or NIR in the case of the SWIR bands). In effect, the simulated uncertainty includes errors from both the atmospheric correction algorithm and the added Gaussian noise in the NIR or SWIR bands. The reflectance uncertainty spectra (from UV to red) are then used for the bio-optical model sensitivity analysis by Stephane Maritorena.

Example Results. Figure 1 provides sample results in the reflectance uncertainty spectra (UV to red or UV to NIR) with simulations from atmospheric correction algorithm using the NIR or

SWIR bands. The error in the normalized water-leaving reflectance, $[\rho_w(\lambda)]_N$, is actually the standard deviation of the derived uncertainty in $[\rho_w(\lambda)]_N$ over the 5000 Gaussian noise realizations, i.e., each point in the plot was derived from 5000 simulations ($[\rho_w(\lambda)]_N$ errors were first obtained with these 5000 simulations and then STD error was derived). The STD error was computed assuming that the mean value = 0 (i.e., error free). Figures 1(a) and 1(b) are results for the NIR atmospheric correction algorithm (using 765 and 865 nm) with the M80 and T80 aerosol models, respectively, while Figures 1(c) and 1(d) are results for the M80 and T80 aerosols using the SWIR atmospheric correction algorithm (with bands of 1240 and 1640 nm) for various SNR values. Note that for the SWIR results (Figures 1(c) and 1(d)), errors in $[\rho_w(\lambda)]_N$ for two NIR bands are also included. Results in Figure 1 show that, as SNR value increases (or noise decreases), error in $[\rho_w(\lambda)]_N$ decreases (as expected), and it reaches the inherent algorithm error (Gordon and Wang, 1994; Wang, 2007).

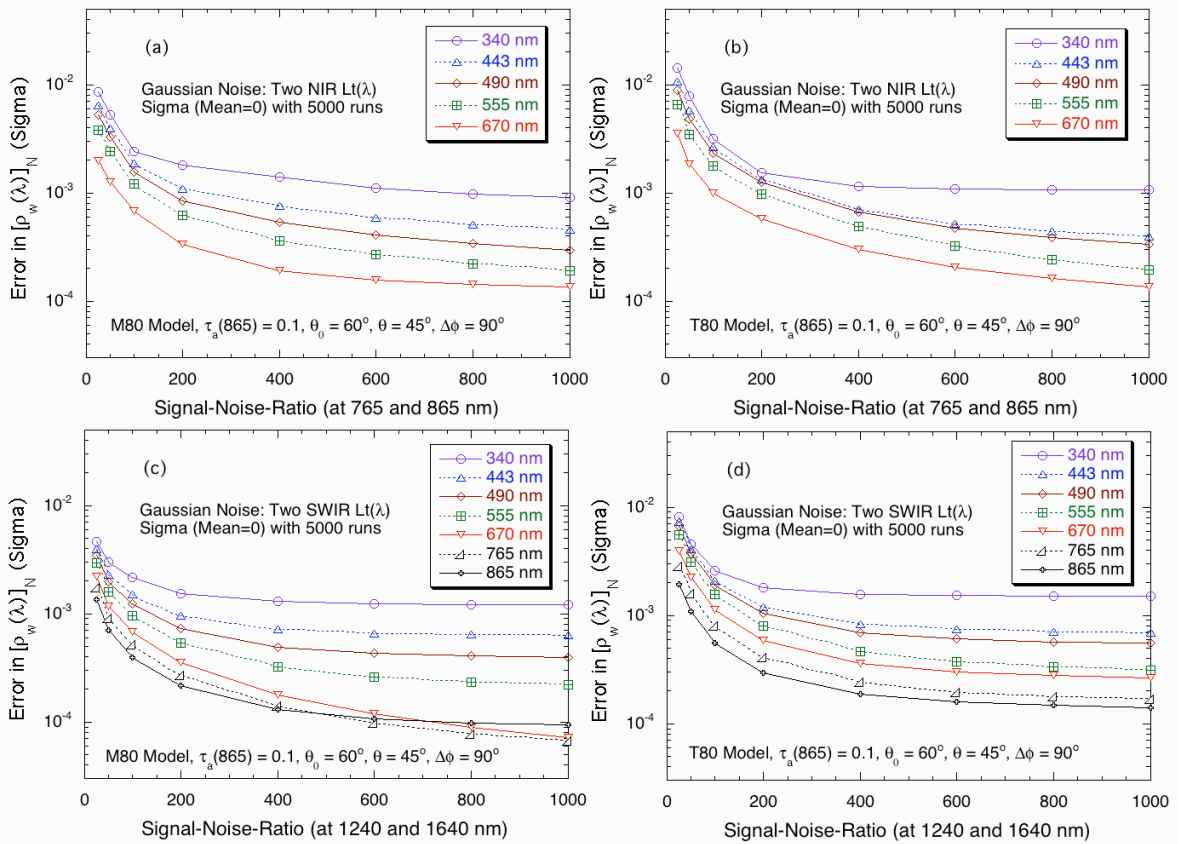


Figure 1. Error in the derived normalized water-leaving reflectance (in standard deviation with the mean value of 0) from 5000 Gaussian noise realizations as a function of the SNR value using the NIR (plots a and b) and SWIR (plots c and d) atmospheric correction algorithms. Aerosol model and AOT value, as well as solar-sensor geometry are indicated in each plot. For the NIR algorithm, error spectra data from UV to red are provided (plots a and b), while for the SWIR algorithm error spectra from UV to NIR are shown (plots c and d).

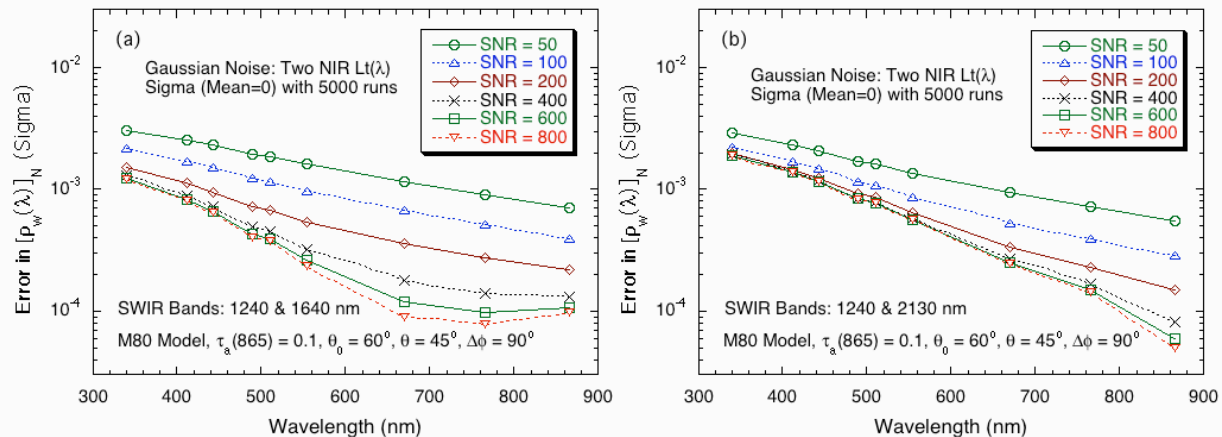


Figure 2. Error in the derived normalized water-leaving reflectance (in standard deviation with the mean value of 0) from 5000 Gaussian noise realizations as a function of the wavelength for various SNR values using the SWIR atmospheric correction algorithm with two SWIR bands of (a) 1240 and 1640 nm and (b) 1240 and 2130 nm. Aerosol model and AOT value, as well as solar-sensor geometry are indicated in each plot.

Figure 2 provides sample results in the reflectance uncertainty spectra as a function of the wavelength (UV to NIR) for various SNR values with simulations from atmospheric correction algorithm using the two SWIR band sets, i.e., 1240 and 1640 nm (Figure 2(a)) and 1240 and 2130 nm (Figure 2(b)). Importantly, results in Figure 2 show that errors in $[\rho_w(\lambda)]_N$ from atmospheric correction are spectrally coherent. In addition, Figure 2 demonstrates that a SNR value between ~ 200 - 300 for the SWIR bands 1240 and 1640 nm is adequate (Figure 2(a)), while for the SWIR band 2130 nm a minimum of SNR value ~ 100 is required. At these SNR values for the SWIR bands, the derived water-leaving reflectance spectra from the SWIR atmospheric correction algorithms almost reach their corresponding algorithm inherent accuracy. It should be noted that, however, with even higher SNR values the derived $[\rho_w(\lambda)]_N$ at the red and NIR bands can be further improved.

Summary. Atmospheric correction and bio-optical simulations (see results from Stephane Maritorena) suggest that (1) for the NIR bands a minimum SNR value of ~ 600 is required, and (2) for the SWIR bands at 1240 and 1640 nm a minimum SNR value of ~ 200 - 300 is required, while for the 2130 nm band a minimum SNR value of ~ 100 is adequate.

(3) Bio-optical model sensitivity analysis

Simulations were performed to assess how noise in the spectral marine remote sensing reflectance, $R_{rs}(\lambda)$, affects the retrievals of biogeochemical variables from a semi-analytical ocean color model (GSM01, Maritorena et al., 2002). These analyses were performed in order to assess the required SNRs in the ACE visible bands to ensure accurate bio-optical retrievals. Noise is created from the at-sea-level atmosphere reflectance spectra derived from the

atmosphere specific simulations ran by Menghua Wang. The spectral atmospheric noise is added to a marine reflectance spectrum at the surface derived from a chlorophyll-based model (Morel and Maritorena, 2001). We compared the model retrievals obtained when spectral reflectance is contaminated by noise to those retrieved from noise-free spectra. These simulations were run for a variety of atmospheric and marine conditions. This is briefly described below.

Two main kinds of noise were considered: 1) Atmospheric noise caused by errors in the NIR bands and propagated to the visible bands and, 2) noise as a random, spectrally uncoherent fraction of the Top-of-Atmosphere (TOA) reflectance in addition to the NIR created noise. This latter case was designed to represent radiometric noise from other sources than the NIR bands (e.g. calibration). These two cases, will be referred to as "NIR" and "radiometric" errors, respectively.

In all runs, the "pure" marine Rrs signal (= no noise) is generated from the MM01 model (Morel & Maritorena, 2001) for 10 chlorophyll concentration (CHL) values in the 0.02-5 mg/m³ range (400-700 nm every 5 nm). The GSM01 retrievals from the inversion of these "no noise" spectra are the reference to which the "noisy" NIR and radiometric cases are compared.

For the "NIR" errors case, the at-sea-level reflectance spectra caused by errors in the NIR bands (from Menghua Wang) are converted to Rrs, Rrs_NIR(λ), and added to a MM01 marine spectrum, Rrs_MM01(λ , CHL), so

$$Rrs(\lambda, \text{ocean}) = Rrs_MM01(\lambda, \text{CHL}) + Rrs_NIR(\lambda)$$

The resulting spectrum, Rrs(λ , ocean), is then inverted in GSM. The three GSM retrievals (CHL, CDM, BBP) are then compared to the "no noise" case for 5000 spectra for each combination of SNR (8 values), AOT(865) and atmospheric model (2 models) and marine Rrs(λ) (10 spectra). The comparisons are expressed in terms of the %rms for each of the GSM01 product and at each Chl level used to generate the marine Rrs. The %rms is defined as rms*100/reference (reference = retrieval in the no noise case).

For the "radiometric" errors case, a random, Gaussian, spectrally uncoherent fraction of a TOA signal is added to the marine spectra created similarly to what is described in the "NIR" case above. First, TOA signals are constructed for a black ocean with the M80 and T80 models, AOT(865) = 0.1 and for solar, sensor, and relative azimuth angles of 60, 45, and 90 degrees, respectively. The ocean contribution to the TOA signal is calculated as a MM01 reflectance spectrum transmitted through the atmosphere (with transmittance values matching the atmospheric model and geometry and AOT(865) of 0.05, 0.1, 0.2, and 0.3) and is added to the atmospheric TOA component (converted to Rrs units; Rrs_TOA(λ)). The fraction of the TOA signal that is added to the marine spectrum created as in the NIR cases is determined through the generation of random Gaussian numbers with a mean of 0 and a standard-deviation of 1/SNR(visible) with SNR(visible) set to 10., 20., 40., 100., 200., 400., 800., 1000. and 2000. Then, each wavelength of the TOA spectrum is multiplied by a unique random number (rn) and that fraction of the TOA spectrum is added to the other components of the marine signal. This is done independently for each of the 5000 spectra corresponding to each SNR(NIR)/AOT(865)/atmospheric model combination used in the atmosphere simulations. In

summary, in the "radiometric" errors case the at-sea-level Rrs is generated as:

$$Rrs(\lambda, \text{ocean}) = Rrs_MM01(\lambda, \text{CHL}) + Rrs_NIR(\lambda) + (Rrs_TOA(\lambda) * m(\lambda, \text{SNR}(\text{visible})))$$

By looking at how much the retrievals from the noisy reflectance spectra depart from those derived without addition of noise, it is possible to assess the SNR(visible) value that allows an acceptable accuracy in the retrievals. It should be mentioned that in this approach, we assume an identical SNR level throughout the visible spectrum and does not take into account the fluorescence bands. Figures 3 and 4 illustrate the results of these analyses.

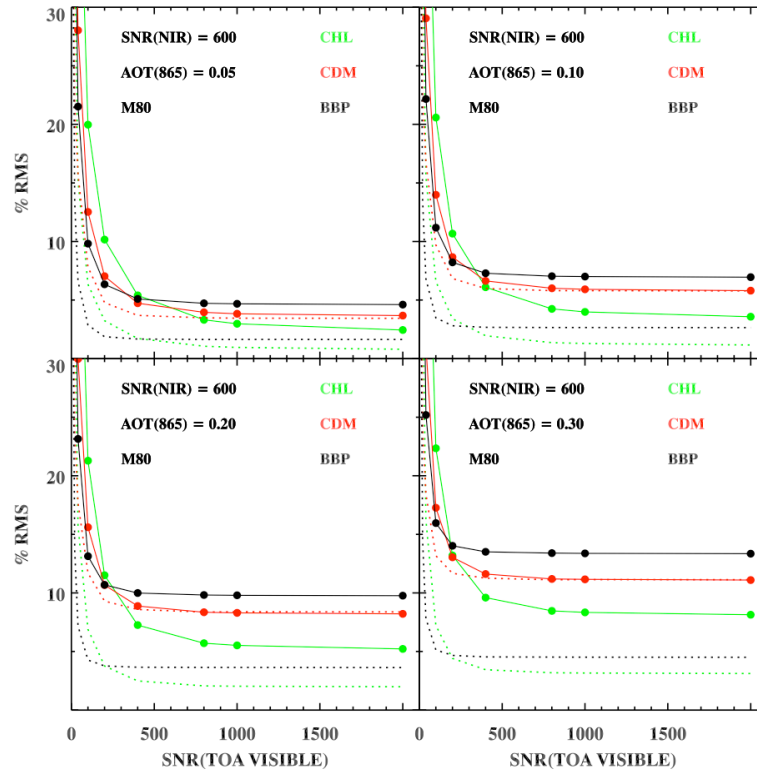


Figure 3. Example of the average (solid lines and symbols) and standard-deviation (dotted lines) of the %rms error over the full range of CHL values used as input in MM01 for the 3 GSM01 retrievals (green: CHL, red: CDM, black: BBP) as a function of the SNR values in the visible and for SNR(NIR)=600 and different AOT(865) values.

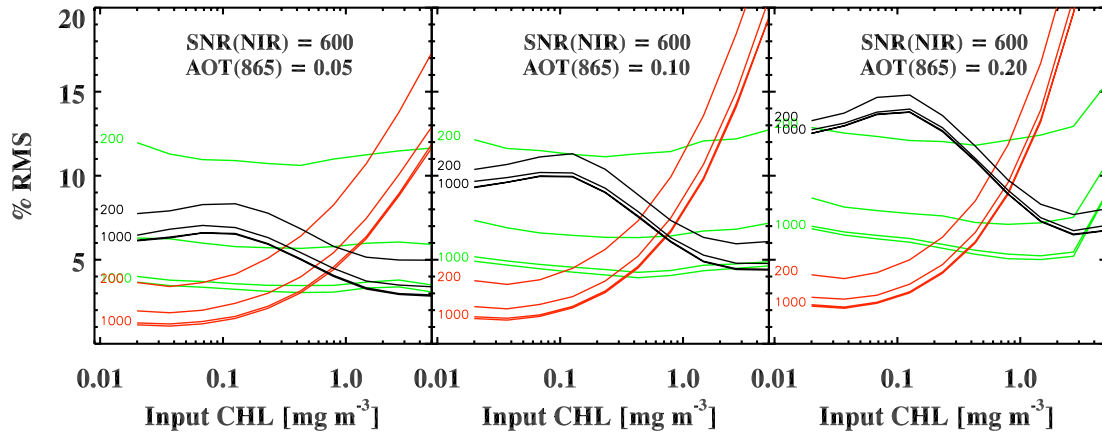


Figure 4. Example of the %rms error for each of the GSM01 retrievals (green: CHL, red: CDM, black: BBP) as a function of the CHL values used as input in MM01 for SNR(NIR)= 600 and different AOT(865) values. For each retrieval, the curves for SNR(visible) of 200, 400, 800 and 1000 are plotted, the highest (=1000) and lowest (=200) SNR(visible) values are indicated at either the beginning or the end of each curve.

For the minimum SNR(NIR) value of 600 suggested above, Figure 4 shows that for the three GSM retrievals the errors become stable in the 800-1000 SNR(vis) range (CHL gets stable at higher SNRs than the other 2 retrievals). The mean error (for the full range of CHL values used as input into MM01) remains under 10% for the clear atmosphere cases only ($AOT(865) \leq 0.1$). This is confirmed in Figure 3 where the errors in the GSM retrievals stay under or close to 10% (except for CDM in eutrophic waters) for clear atmospheres and high SNRs. For the visible bands, a minimum SNR of ~1000 is thus recommended.

Table 1 in the main text summarizes the SNR requirement for atmospheric and science bands. In this table, the SNR value at 350 nm is lower than in the other UV bands because its application is assumed to be dedicated to detecting absorbing aerosols, which does not require a value of 1000. The SNR at 678 nm is set at 1400 based on analysis of MODIS retrievals (the bio-optical sensitivity analyses above did not include fluorescence line height).

References for Sections 2 and 3

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