

Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) mission

PACE Science Data Product Validation Plan



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1 INTRODUCTION

1.1 Purpose

NASA's Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) mission will make global ocean color and atmospheric measurements to provide extended data records on ocean ecology and global biogeochemistry, along with polarimetry measurements to provide advanced systematic observations of aerosols, clouds and the ocean. Fundamental to the success of any Earth Science space-borne mission is the capability to assess and verify the in-orbit quality of the data products generated and distributed by that mission. Herein, the term “validation” is used to refer to this data quality performance assessment and verification process. The scientific community has adopted various approaches to collect field (or *in situ*) measurements coincident (or nearly coincident in time and space) with the satellite observations with which to conduct matchup comparisons and estimate the uncertainties or deviations between the field measurement and satellite derived data product in question. This document describes the plan for the validation of threshold (required) and advanced (goal) data products to be produced by the PACE Project from the Ocean Color Instrument (OCI) and the two polarimeters, HARP2 and SPEXone.

1.2 Mission Requirements Overview Pertaining to the PACE Validation Program

The PACE Program Level Requirements Agreement (PLRA) and Mission Requirements Document (MRD) among other documents (see section 1.5) provide the requirements pertaining to the PACE Science Data Product Validation Program. The PLRA and MRD specify that *“post-launch field validation work is required to evaluate the PACE science data products in Tables 1 and 2 within 12 months of commissioning. The PACE validation programs (provided by HQ PACE Science) shall include the following for the mission duration:*

- a) *Shipboard and aircraft campaigns as required to collect the data products defined in Tables 1 and 2.*
- b) *Autonomous instrument systems that collect continuous records of any of the individual data products defined in Tables 1 and 2.”*

Noting that the table numbering in the previous quote applies to both the PLRA and to this document. The Headquarters (HQ) PACE Program Science is responsible for the competed science teams and validation systems(s), which includes the PACE Validation Science Team (PVST) [see PLRA p. 6]. Both PACE Project Science and the PACE Science Data Segment (SDS) have formal requirements and responsibilities pertaining to validation efforts. Project Science is responsible for the quality of the PACE science data products and is thus required to perform the validation of the science data products. To accomplish this aim, Project Science selects the science data processing algorithms and provides them to the SDS along with the list of validation data types and sources required to support the science data product validation. The PACE SDS supports the validation effort by performing the science product validation analysis and will interact with Project Science in these efforts. More specifically, the validation-related requirements on the SDS pertain to utilization and augmentation of existing facilities to support validation of PACE science data products, development of protocols, data processing, and quality control of in-water field measurements, perform the ingest, processing, and quality control of field data necessary for validation, delivery of *in situ* validation data to the OB.DAAC,

perform the matchup comparisons of PACE science data with *in situ* measurements as directed by Project Science, and deliver validation results to Project Science for review, further analysis, and public dissemination. The OB.DAAC also contributes to the validation effort through ingestion and archiving of *in situ* measurements and maintenance of SeaBASS and its various software tools that facilitate matchups of *in situ* measurements with PACE science data products.

1.3 Scope

The PACE Science Data Product Validation Plan accomplishes the following:

- Define the objectives of the PACE Science Data Product Validation Program
- Describe the roles of PACE Project Science, Program Science, SDS, science teams including the PACE Validation Science Team in accomplishing the Validation Program
- Identify essential elements of the PACE Science Data Product Validation Program
- Prescribe the attributes of validation sites for *in situ* measurement and sample collections to enable validation of PACE science data products
- Identify the required and advanced data products from all PACE sensors proposed for validation
- Identify required *in situ* measurement and sample collections (both for validation as well as ancillary metadata) necessary to accomplish data product validation along with expected measurement range and required uncertainty
- Introduce a planned PACE airborne and shipborne validation campaign
- Identify other potential sources (external to PACE) of field data that PACE can utilize for validation of data products
- Describe potential augmentations to existing infrastructure to enable validation of PACE Science Data Products
- Describe the approaches for validation of PACE science data products

This plan does not prescribe the PACE validation activities, prioritize efforts for collection of *in situ* measurements, describe the details of how each particular data product will be validated, the protocols for field measurement collections, nor how the PACE program science resources for validation will be allocated. The PACE Science Data Product Validation program will be a best effort activity. Ultimately, the full scope of the PACE Science Data Product validation effort may be constrained by the limited set of matchup data available, i.e., coincident PACE science data products with corresponding *in situ* measurements.

1.4 PACE Mission Overview

The Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) mission is a strategic climate continuity mission that was defined in the 2010 document *Responding to the Challenge of Climate and Environmental Change: NASA's Plan for Climate-Centric Architecture for Earth Observations and Applications from Space* (referred to as the "Climate Initiative"). The Climate Initiative complements NASA's implementation of the National Research Council's Decadal Survey of Earth Science at NASA, NOAA, and USGS, entitled *Earth Science and Applications from Space: National Imperatives for the Next Decade and Beyond*.

PACE will extend the high quality ocean ecological, ocean biogeochemical, cloud, and aerosol particle data records begun by NASA in the 1990s, building on the heritage of the Sea-Viewing

Wide Field-of-View Sensor (SeaWiFS), the Moderate Resolution Imaging Spectroradiometer (MODIS), the Multi-angle Imaging SpectroRadiometer (MISR), and the Visible Infrared Imaging Radiometer Suite (VIIRS). The mission will be capable of collecting radiometric and polarimetric measurements of the ocean and atmosphere, from which these biological, biogeochemical, and physical properties will be determined. PACE data products will not only add to existing critical climate and Earth system records, but also answer new and emerging advanced science questions related to Earth's changing climate.

PACE is classified as a Category 2 mission, per the criteria in NASA Procedural Requirement (NPR) 7120.5E, NASA Space Flight Program and Project Management Requirements. The mission classification is C according to NPR 8705.4B, Risk Classification for NASA Payloads.

The PACE observatory is comprised of three instruments, an Ocean Color Instrument (OCI) and two polarimeters, the Hyper-Angular Rainbow Polarimeter 2 (HARP2) and the Spectro-Polarimeter for Exploration (SPEXone). The OCI is the primary instrument on the observatory and is being developed at Goddard Space Flight Center (GSFC). The OCI is a hyper-spectral scanning (HSS) radiometer designed to measure spectral radiances from the ultraviolet (UV) to shortwave infrared (SWIR) to enable advanced ocean color and heritage cloud and aerosol particle science. The HARP2 and SPEXone are secondary instruments on the PACE observatory, acquired outside of GSFC. The Hyper-Angular Rainbow Polarimeter instrument (HARP2) is a wide swath imaging polarimeter that is capable of characterizing clouds and atmospheric aerosols for purposes of sensor atmospheric correction as well as atmospheric science. The SPEXone provides highly accurate atmospheric aerosol and cloud products that extend into the UV spectral range of relevance to OCI, but over a narrower swath than OCI and HARP2,

This three-instrument PACE mission has the following multiple scientific goals:

- Extending key systematic ocean biological, ecological, and biogeochemical climate data records and cloud and aerosol climate data records;
- Making global measurements of ocean color data products that are essential for understanding the global carbon cycle and ocean ecosystem responses to a changing climate;
- Collecting global observations of aerosol and cloud properties, focusing on reducing the largest uncertainties in climate and radiative forcing models of the Earth system; and,
- Improving our understanding of how aerosols influence ocean ecosystems and biogeochemical cycles and how ocean biological and photochemical processes affect the atmosphere.

The PACE satellite is planned for a launch in 2022-2023. The PACE project office at NASA's GSFC is responsible for the satellite development, launch and operations. The mission is planned for launch into a Sun synchronous polar orbit at 676.5 km with an inclination of 98 degrees and a 1 pm local ascending node crossing time. The spacecraft bus will host the OCI, HARP2, and SPEXone instruments. The GSFC PACE Project office will oversee the mission and the development of the satellite, launch vehicle, mission operations control center, and operations. The Headquarters Program Science will separately fund the science data processing

system and competed science teams, which will include field-based vicarious calibration and data product validation efforts to support the Project science team.

NASA Headquarters has directed the mission development to be guided by a Design-to-Cost (DTC) process. All elements of the mission, other than the cost, are in the DTC trade space. At the heart of the DTC process are the mission studies, performed across all the mission elements. The mission studies will be used to define appropriate approaches within and across elements while maximizing science capabilities at a high cost confidence. Mission baseline requirements development is also embedded within the DTC process, as these requirements were not established at the onset of the mission concept development. Baseline mission requirements will be a product of the mission studies and will be defined by the project office as part of the DTC process.

The PACE mission consists of four major segments: space segment (SS), ground segment (GS), science data segment (SDS), and the launch segment (LS).

- The space segment consists of the spacecraft bus, the OCI, and two polarimeters. The spacecraft and OCI are being developed and integrated at GSFC. The polarimeters are contributed instruments. The spacecraft and instruments will be integrated as the PACE observatory at GSFC.
- The GS and associated Mission Operations Center (MOC) will be developed, integrated, and operated at GSFC. The GS provides for the command and control and health and safety monitoring of the PACE observatory on-orbit, as well as ensuring the science data are accounted for and delivered to the SDS. The MOC will house the flight operations team (FOT) and is being managed by the PACE project through observatory commissioning. After commissioning, the FOT will be managed by the GSFC Earth Science Mission Operations (ESMO) project. The MOC performs all real time operations and off-line operations functions, including planning and scheduling, orbit and attitude analysis, housekeeping telemetry data processing, monitoring/managing the spacecraft and instruments, first line health/safety for the instruments, and housekeeping archiving and analysis.
- The SDS will be located at GSFC, but managed (separately from the project) by the NASA Headquarters Earth Sciences Division and its GSFC designee. The SDS will ingest, apply calibration and science algorithms, and process the science data, provide science software development and algorithm integration, act as the science data interface to the science team, and deliver all science data products to the NASA-assigned Distributed Active Archive Center (DAAC).
- The LS is planned for a launch vehicle to be selected and procured by the NASA Launch Services Program at Kennedy Space Center (KSC).

In addition to utilizing GSFC institutional capabilities, the project will utilize the NASA institutional capabilities at GSFC such as the Flight Dynamics Facility (FDF), Near Earth Network (NEN), Ocean Biology Processing Group (OBPG), Space Network (SN), and NASA Integrated Services Network (NISN). PACE plans to generate 3.5 Terabits of science data daily. The data are downlinked from the observatory during 12-14 daily contacts via Ka-band

communications to the NEN's ground stations. The observatory will also receive ground commands and transmit real-time housekeeping telemetry via an S-band 2-way link through the NEN during nominal operations. The observatory also has the capability of receiving ground commands and transmitting real-time housekeeping telemetry, via S-Band, through the SN during critical or contingency operations.

1.5 Related Documentation

1. PACE Program Level Requirements Agreement (PLRA), PACE-SYS-REQ-0007 (final version to be released on the PACE website by early 2021).
2. PACE Mission Requirements Document (MRD), PACE-SYS-REQ-0019 (final version to be released on the PACE website by early 2021).
3. NASA Earth Science Data Systems (ESDS) Program Data and Information Policy, <https://earthdata.nasa.gov/earth-science-data-systems-program/policies/data-information-policy>
4. Pre-Aerosol, Clouds, and ocean Ecosystem (PACE) Mission Science Definition Team (SDT) Report, NASA/TM-2018-219027/Vol. 2
https://pace.oceansciences.org/docs/PACE_TM2018-219027_Vol_2.pdf

2 PACE SCIENCE DATA PRODUCT VALIDATION PROGRAM

The overarching goal of the PACE Science Data Product Validation program is to verify that the required and advanced science data products from OCI, HARP2, and SPEXone meet the specified mission requirements and goals and to provide an evaluation of uncertainty for each data product. Assessment of OCI threshold science data products remains a mission requirement. Assessment of HARP2 and SPEXone science data products and OCI advanced products will be pursued on a best-effort basis.

PACE will deliver the most comprehensive suite of combined measurements of global ocean color, aerosols and clouds in NASA's history (Werdell et al., 2019). Among several science objectives, PACE will extend key systematic ocean ecological and biogeochemical, cloud and aerosol climate data records. As such, these data products will be used to study the impacts of climate forcing and human-induced change within the Earth's ocean ecosystems and how aerosols and clouds influence and respond to climate change. Thus, a well-planned and executed science validation program is essential to the success of PACE. In addition to verifying that data products meet mission performance requirements, it is also necessary to assess the uncertainties associated with each data product and how they vary across ocean water types, complexity in cloud properties, and aerosol loading and composition. Customarily, validation of satellite data products has been accomplished by comparing satellite data with measurements collected *in situ* and through airborne or independent remote sensing platforms, such as another satellite sensor or instrumented system on the Earth's surface. The validation analysis involves comprehensive statistical comparisons of field measurements (*in situ* or remotely sensed) that are coincident (or nearly coincident) with the satellite data products to determine the uncertainties or deviations between the field measurements and satellite derived data products. An essential element for any such validation analysis is that the uncertainties of the field measurements must be well understood and quantifiable. This requires development and strict adherence to community accepted field measurement protocols that describe proper traceability to fiducial references. In lieu of field measurements (aircraft/ship/ground), which may prove elusive or difficult to obtain for certain PACE science products, validation of such PACE data products may be accomplished using previously validated data products produced from other satellite sensors (e.g., VIIRS).

The primary objectives of the PACE Science Data Product Validation Program are to:

- Verify that PACE OCI, HARP2 and SPEXone threshold and advanced data products meet mission-specified requirements
- Rigorously assess uncertainties in PACE threshold and advanced science data products; and,
- Validate uncertainty estimates across major ocean water types and meaningful ranges of cloud conditions, aerosol types and loadings.

2.1 Historical Perspective

2.1.1 Ocean Optics, Ecology and Biogeochemistry

The ocean optics, ecology and biogeochemistry communities have several decades of experience with validation of ocean color satellite products beginning with the Coastal Zone Color Scanner (CZCS) in the late 1970's (e.g., Hovis, 1982), SeaWiFS starting in 1997, the two MODIS

instruments on Terra (2000) and Aqua (2002), MERIS on ESA's ENVISAT (2002), GOCI (2010), and VIIRS on Suomi-NPP (2011). Arguably the most successful ocean color validation activity to date was work conducted under the Sensor Intercomparison for Marine Biological and Interdisciplinary Ocean Studies (SIMBIOS) program (McClain et al., 2002). The techniques for performing validation exercises are well-established (Bailey and Werdell, 2006). A number of validation-enabling activities and support services were also implemented through the SeaWiFS project and SIMBIOS program including the development of: (1) community consensus field measurement protocols (Mueller et al., 2003); (2) field instrument technologies and calibration instruments; (3) a field instrument pool; (4) a field measurement database (SeaWiFS Bio-optical Archive and Storage System; SeaBASS; Werdell and Bailey, 2005); (5) field instrument intercalibrations and measurement round robins; (6) public-facing tools that provide satellite sensor overflight predictions for field sampling sites; (7) distribution tools for near real time ocean color imagery; (8) web-based satellite data distribution; (9) publicly available satellite data processing software (SeaDAS); (10) support for sun photometers on coastal Aerosol Robotic Network (AERONET; Holben et al., 1998) sites for atmospheric correction evaluation; and (11) deployment of handheld sun photometers on research ships (Fargion et al., 2001; Knobelspiesse et al., 2003; Knobelspiesse et al., 2004). The sunphotometer deployment on coastal AERONET sites was a precursor to the establishment of ocean color AERONET sites (AERONET-OC) with the addition of SeaPRISM above-water radiometric sensors, which were implemented to validate water-leaving reflectance of various ocean color satellite sensors (Hooker et al., 2000; Zibordi et al., 2010). Likewise, handheld sun photometer deployment was a predecessor to the Maritime Aerosol Network (MAN; Smirnov et al., 2009) component of AERONET.

2.1.2 Aerosols and Clouds

The gold standard for satellite aerosol property measurements (aerosol optical depth [AOD], Ångström exponent, and in some cases properties such as fine mode AOD fraction) is sun photometry, with AERONET and the MAN being the most widely-used networks for land/coast/island and open-water validation respectively. This is due to a combination of their standardized instrumentation and data processing/distribution systems, well-understood uncertainties, and broad coverage of key aerosol/surface regimes. These uncertainties are typically several times smaller than the uncertainty on the satellite retrievals (e.g., Eck et al., 1999; Dubovik et al., 2000). The techniques for performing validation exercises are also well-established, with most using a spatio-temporal averaging approach outlined by Ichoku et al. (2002) to minimize the contributions from true variability in the underlying aerosol field to the matchup uncertainty.

The bulk of satellite cloud property evaluation consists of intercomparisons of various aspects against other satellite data products to assess consistency (e.g. Holz et al., 2008; Marchant et al., 2016; Karlsson and Devasthale, 2018), rather than routine true validation against a reference ground truth. The cloud retrieval problem is in some senses more complicated than that for aerosols or ocean color, due to the higher spatial and temporal variability of cloud cover, retrieval sensitivity to vertical and horizontal inhomogeneity (e.g., Pincus et al., 2012; Marshak et al., 2006), and properties increasing collocation uncertainties (Holz et al., 2008), and well-understood different sensitivities of various satellite measurement types and wavelengths to different cloud properties. For example, the spectral dependence of photon penetration depths leads to expected and quantifiable differences in cloud top height, effective radius, and water

path from different sensors, due to real vertical structure in clouds (e.g., Platnick, 2000; Sayer et al., 2011).

Despite this, ground sites with various combinations of instrumentation and field campaigns are able to provide useful validation data for various cloud properties. Quantities such as effective radius can be validated against cloud probes (Witte et al., 2018; Ahn et al., 2018). Both ground-based and spaceborne lidar, radar and microwave sensors in various combinations can be used to validate cloud detection, phase, altitude, and water path (Ackerman et al., 2008; Wang et al., 2016; Kollias et al. 2019; and Marchand, 2016 for a review). As liquid/ice water path is derived from the phase, optical depth, and effective radius retrievals, this also provides an indirect evaluation of those quantities. Cloud optical depth itself can be derived from upward looking optical measurements (Min et al., 2003), and this approach has been used to validate cloud products from the GOES satellite sensors (Min and Harrison, 1996). Additionally, resources such as AERONET have demonstrated the use of a zenith radiance mode that allows cloud optical depth to be retrieved (Chiu et al., 2010), and this measurement mode could be further refined to include effective radius (Chiu et al., 2012). A fraction of AERONET instruments have sensitivity to linear polarization, which can be utilized to determine cloud thermodynamic phase (Knobelspiesse et al., 2015; Eshelman et al., 2019).

Airborne field campaigns are crucial to provide observations at different spatial and temporal scales than those from ground and orbit. Ideally, they include measurements from remote sensing instruments that can serve as a proxy for the instruments on PACE, and *in situ* measurements of retrieval products. Examples of similar recent campaigns include Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys (SEAC⁴RS, Toon et al., 2016), North Atlantic Aerosols and Marine Ecosystems Study (NAAMES, Behrenfeld et al., 2019) and ObseRvations of Aerosols above CLouds and their intERactionS (ORACLES, Zuidema et al., 2016). Obviously, such field campaigns can provide valuable validation data for ocean science as well (da Silva et al., 2019). Section 2.7 is a notional description of what must be considered when designing a field mission for validation of science data products similar to PACE, and a more complete, stand-alone document on this topic will be created to follow this one.

2.2 Roles in Science Data Product Validation Program

Several entities work collaboratively to collect, submit, evaluate, archive, and distribute field data collections for the purposes of validating the required and advanced PACE Science Data Products (Fig. 1). The following describes the core entities.

Program Science

The Headquarters Program Science shall solicit for a PACE Validation Science Team (PVST), which will be tasked to collect appropriate field measurements, in accordance with best-practice, community accepted protocols (e.g., <https://ioccg.org/what-we-do/ioccg-publications/ocean-optics-protocols-satellite-ocean-colour-sensor-validation/>; Holben et al., 1998; Giles et al., 2019; Smirnov et al., 2009), for the sole purpose of validating required and advanced PACE Science Data Products (Tables 1-4). The Mission Program Scientist and Deputy Program Scientist(s) will facilitate a joint airborne and ship field mission to be executed within several months of the launch of PACE by Project Science and selected members of the PVST.

PACE Validation Science Team

The PACE Validation Science Team (PVST) selected through the ROSES peer-review process will be supported and tasked to collect and analyze field data corresponding to PACE science data products, including related metadata, documentation of protocols, and measurement uncertainties, to enable the validation matchup analysis for evaluation of required and advanced PACE science data products.

Earth Science Data and Information System Project

The Earth Science Data and Information System (ESDIS) Project is a part of the Earth Science Projects Division under the Flight Projects Directorate at GSFC. The ESDIS Project manages the science data systems of the Earth Observing System Data and Information System (EOSDIS). EOSDIS provides science data to a wide community of users through a series of Distributed Active Archive Centers (DAACs). In the context of this Plan, this series of organizations (hereafter referred to as simply ESDIS) maintains responsibility for long-term archival and distribution of science satellite data products from PACE as well as the long-term archival and distribution of the *in situ* science measurements and validation database referred to as SeaBASS. The principal DAAC for PACE is assumed to be the Ocean Biology DAAC (OB.DAAC).

PACE Science Data Segment

The PACE Science Data Segment (SDS) acts similarly to an ESDIS Science Investigator-led Processing System (SIPS) and maintains responsibility for developing the science processing software, implementing science algorithms, generating the associated science data products, and delivering all science data to the NASA-assigned DAAC. The PACE SDS will be supporting the validation matchup analysis for evaluation of required and advanced PACE science data products under the direction of PACE Project Science. Furthermore, the SDS shall develop protocols and methods for measurement, processing, and quality control of required and advanced in-water *in situ* measurements.

Project Science

Project Science at GSFC evaluates and assesses the performance of PACE science data product validation provided by SDS, PVST or other contributors and uses this information in making decisions on science data product validation status and guidance to SDS on science data product processing and distribution.

Contributors

Contributors provide and analyze field data corresponding to PACE science data products, including related metadata, documentation of protocols, and measurement uncertainties, to enable the validation matchup analysis for evaluation of required and advanced PACE science data products. Contributors may include the PACE Project Science Team, competitively-selected PACE science team members, and collaborators in the domestic and international science and user community.

External *in situ* data contributors

External *in situ* data resources are those supported by NASA, other U.S. agencies, and international agencies.

Science Validation Program Operations Board

A Science Validation Operations Board (SVOB) provides overall guidance and oversight for the science data product validation program described in this Plan. The SVOB is responsible for planning and coordinating any directed validation airborne-ship field campaign(s). For PACE, this SVOB will consist of the Project Scientist, Deputy Project Scientists, Mission Program Scientist, Deputy Program Scientist(s), SDS Manager, OB.DAAC Manager, and an ESDIS Program representative. The SVOB will also interact with PVST members conducting validation efforts separate from the directed validation airborne-ship field campaign(s).

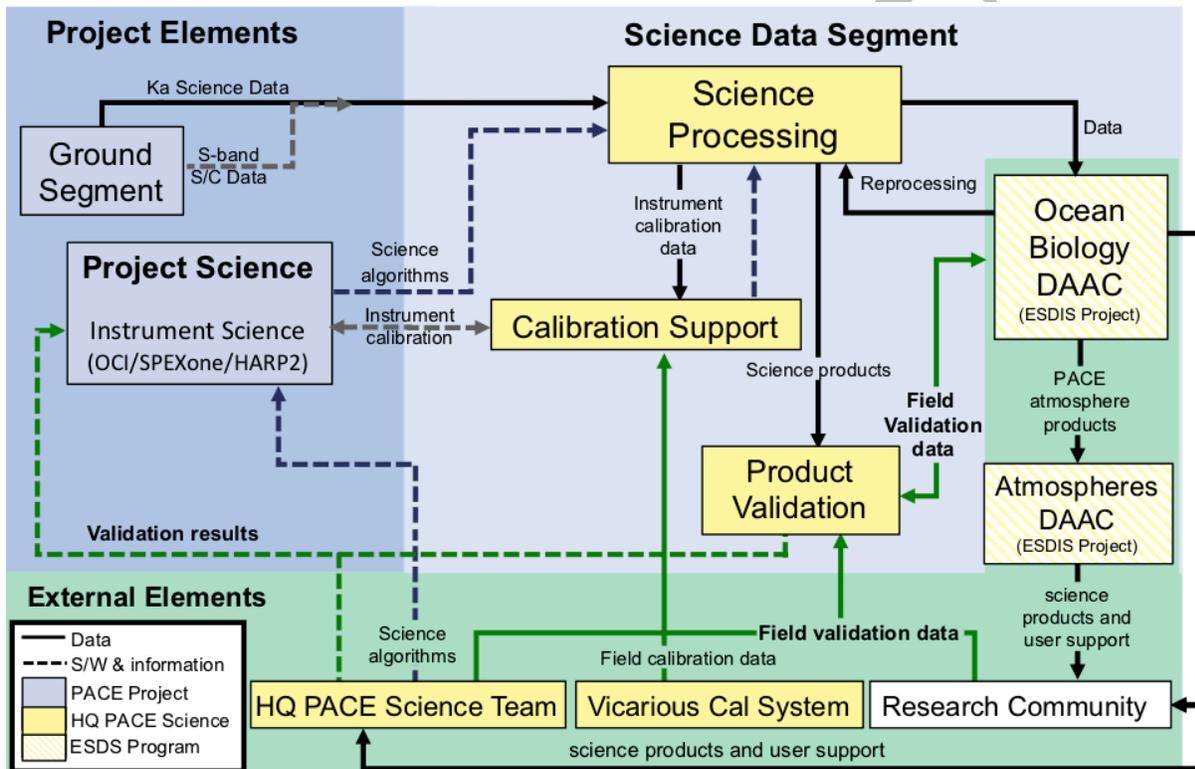


Figure 1. PACE validation program interfaces and data flow.

2.2.1 Interactions between the Project and PVST

PACE Project Science and Science Data Segment members will interface with the awarded PACE Validation Science Team(s) for implementation of validation activities, evaluation of data collection efforts including field protocols and data processing, and assessment of PVST data quality. Project Science and SDS designees will participate in PVST activities, including scientific discussions, planning of field efforts, measurement discussions, and data processing associated validation activities. This will be done to resolve any outstanding issues including, but not limited to, data transfers, data formats, data processing and post-processing strategies, sharing of software, and acceptable data collection and quality-controlled data submission latencies.

2.2.2 Data and Information Policy

Each entity working under the auspices of PACE (Project Science, SDS, Science Teams, etc.) will adhere to the NASA data policy:

“NASA's Earth Science Data Systems (ESDS) Program was established to use the advanced technology of NASA to understand and protect our home planet by using our view from space to study the Earth system and improve prediction of Earth system change. To meet this challenge, NASA promotes the full and open sharing of all data with the research and applications communities, private industry, academia, and the general public. The greater the availability of the data, the more quickly and effectively the user communities can utilize the information to address basic Earth science questions and provide the basis for developing innovative practical applications to benefit the general public.”

The full ESDS Data and Information Policy is available at <https://earthdata.nasa.gov/earth-science-data-systems-program/policies/data-information-policy>.

2.3 PACE Science Data Products

2.3.1 Required Science Data Products

Post-launch field validation work is required to evaluate the PACE science data products listed in Tables 1 and 2 within 12 months of commissioning. As stated previously, the PACE validation programs (provided by HQ PACE Science) shall include the following for the mission duration:

- a) Shipboard and aircraft campaigns as required to collect the data products defined in Tables 1 and 2.
- b) Autonomous instrument systems that collect continuous records of any of the individual data products defined in Tables 1 and 2.

Tables 1 and 2 present baseline science requirements for key heritage, systematic ocean biological, ecological, and biogeochemical data records and cloud and aerosol data records to be produced by OCI. These key data records extend heritage capabilities (e.g., from the Sea-viewing Wide Field-of-view Sensor (SeaWiFS); Moderate Resolution Imaging Spectroradiometer (MODIS); and Visible Infrared Imaging Radiometer Suite (VIIRS)).

Table 1. Required OCI ocean color data products.

Data Product	Baseline Uncertainty
Water-leaving reflectances centered on (± 2.5 nm) 350, 360, and 385 nm (15 nm bandwidth)	0.0057 or 20%
Water-leaving reflectances centered on (± 2.5 nm) 412, 425, 443, 460, 475, 490, 510, 532, 555, and 583 (15 nm bandwidth)	0.0020 or 5%
Water-leaving reflectances centered on (± 2.5 nm) 617, 640, 655, 665 678, and 710 (15 nm bandwidth, except for 10 nm bandwidth for 665 and 678 nm)	0.0007 or 10%
Ocean Color Data Products to be Derived from Water-leaving Reflectances	
Concentration of chlorophyll-a	
Diffuse attenuation coefficients 400-600 nm	
Phytoplankton absorption 400-600 nm	
Non-algal particle plus dissolved organic matter absorption 400-600 nm	
Particulate backscattering coefficient 400-600 nm	
Fluorescence line height	

The requirements for ocean color products stated in Table 1 are defined for 50% or more of the observable deep ocean (depth > 1000 m).

Table 2. Required OCI aerosol and cloud data products.

Data Product	Range	Baseline Uncertainty
Total aerosol optical depth at 380 nm	0.0 to 5	0.06 or 40%
Total aerosol optical depth at 440, 500, 550 and 675 nm over land	0.0 to 5	0.06 or 20%
Total aerosol optical depth at 440, 500, 550 and 675 nm over oceans	0.0 to 5	0.04 or 15%
Fraction of visible aerosol optical depth from fine mode aerosols over oceans at 550 nm	0.0 to 1	$\pm 25\%$
Cloud layer detection for optical depth > 0.3	NA	40%
Cloud top pressure of opaque (optical depth > 3) clouds	100 to 1000 hPa	60 hPa
Optical thickness of liquid clouds	5 to 100	25%
Optical thickness of ice clouds	5 to 100	35%
Effective radius of liquid clouds	5 to 50 μm	25%
Effective radius of ice clouds	5 to 50 μm	35%
Atmospheric data products to be derived from the above		
Water path of liquid clouds		
Water path of ice clouds		

The requirements in Table 2 are defined for 65% or more of the observable atmosphere. Each requirement is defined as the maximum of the absolute and relative values when both are provided. Table 2 represents threshold aerosol and cloud data products, all of which can be produced by OCI alone.

2.3.2 Advanced Science Data Products

Tables 3 and 4 present examples of advanced science data products to be produced by OCI, HARP2, and/or SPEXone on a best-effort basis. These tables are not exhaustive; they will evolve with time as scientific advances progress. The PACE SDT report (2018) provides additional details and desired science data products.

Table 3. Examples of advanced OCI ocean color, aerosol, and cloud data products.

Advanced ocean data products to be derived from required/advanced OCI data products	Range *
Particulate organic carbon concentration	15 - 2,000 mg m ⁻³
Coastal dissolved organic carbon concentration	50-800 mmol m ⁻³
Particulate inorganic carbon	1.2 x 10 ⁻⁵ - 5.3 x 10 ⁻⁴ mol m ⁻³ 0 - 6.5E ⁻⁴ mg m ⁻³ #
Suspended particulate matter	25 - 70,000 mg m ⁻³
Vertical carbon flux	TBD
Phytoplankton photosynthetic pigments concentrations	TBD
Phytoplankton photoprotective pigments concentrations	TBD
Phytoplankton community composition (on basis of Phyto_C, %total chlorophyll, biovolume)	TBD
Fluorescence quantum yield	TBD
Net primary production	55 - 8,500 mg m ⁻² d ⁻¹
Colored dissolved organic matter absorption coefficient	<i>a</i> _{CDOM(443)} : 0.002 - 0.9 m ⁻¹
Photosynthetically Available Radiation (PAR)	Instantaneous: 0 - 2,200 μmol quanta m ⁻² s ⁻¹ 24-hr flux: 0 - 70 mol quanta m ⁻² d ⁻¹
Phytoplankton carbon (C _{phyto})	TBD
Advanced aerosol data products to be derived from required and advanced OCI data products	
Fraction of visible aerosol optical depth from fine mode aerosols over land at 550 nm	0 to 1
Aerosol Ångström exponent over land	-0.5 to 3
Aerosol Ångström exponent over water	-0.5 to 3
Aerosol effective altitude over land	0 to 8 km
Aerosol effective altitude over water	0 to 8 km
UV absorbing aerosol index	-1 to 20
Advanced cloud data products to be derived from required and advanced OCI data products	
None	

* source: PACE SDT Report, 2018

Values from *in situ* SeaBASS validation data matchups; <https://seabass.gsfc.nasa.gov/>

Table 4. Examples of advanced SPEXone and HARP2 aerosol, cloud, and ocean data products.

Advanced aerosol Multi-Angle Polarimetry data products	Range
Total aerosol optical depth at 380 nm	0.0 to 5
Total aerosol optical depth at 440, 500, 550 and 675 nm over land	0.0 to 5
Total aerosol optical depth at 440, 500, 550 and 675 nm over oceans	0.0 to 5
Total aerosol optical depth at 440, 500, 550 and 675 nm over liquid clouds	0.0 to 5
Fraction of visible aerosol optical depth from fine mode aerosols over oceans at 550 nm	0 to 1
Fraction of visible aerosol optical depth from fine mode aerosols over land at 550 nm	0 to 1
Aerosol Ångström exponent over land	-0.5 to 3
Aerosol Ångström exponent over water	-0.5 to 3
UV absorbing aerosol index	-1 to 20
Aerosol and Cirrus detection	NA
Effective aerosol layer altitude	1 to 9 km
Aerosol effective radius (two modes)	0 to 5µm
Aerosol effective variance (two modes)	0.1 to 0.5
Aerosol sphericity characterization	0 to 1
Aerosol concentration (two modes)	0 to 25
Aerosol absorption optical depth (spectral, two modes)	0 to 2
Single scattering albedo (spectral, two modes)	0 to 1
Refractive index/Real (spectral, two modes)	1.3 to 1.7
Advanced cloud Multi-Angle Polarimetry data products	
Cloud layer detection	NA
Cloud top pressure of opaque (optical depth > 3) clouds	100 to 1000 hPa
Multiple cloud layer detection	NA
Optical thickness of liquid clouds	5 to 100
Optical thickness of ice clouds	5 to 100
Effective radius of liquid clouds	4 to 50 µm
Effective variance of liquid clouds	0.01 to 0.5
Ice crystal roughness	0 to 0.7
Ice crystal aspect ratio	1 to 20
Effective radius of ice clouds*	4 to 50 µm
Water path of liquid clouds (derived from products above)	TBD
Water path of ice clouds (derived from products above)	TBD
Advanced ocean Multi-Angle Polarimetry data products	
Surface ocean wind vectors	TBD
Water-leaving reflectances	TBD
Particle size distribution	TBD
Bulk refractive index	TBD
Scattering coefficient	TBD
Ratio of attenuation to absorption	TBD

*Advanced product would use ice crystal roughness and aspect ratio in OCI size retrieval.

2.4 Tentative timeline of the PACE validation program

The timeline for validation program activities is as follows:

- January-December 2020: SDS in coordination with Project Science begins to ingest *in situ* data from various sources that can be applied to validate PACE required and advanced science data products (see Table 6) for the purpose of preparing for PACE launch and implementation of formal validation activities.
- January 2021: Citations or URL links to field measurement protocols for required and advanced data products (as appropriate) are posted on the PACE website.
 - SDS develops and updates ocean field measurement protocols through post-launch. The most recent versions of the IOCCG Ocean Optics and Biogeochemistry Protocols for Satellite Ocean Colour Sensor Validation available at <https://ioccg.org/what-we-do/ioccg-publications/ocean-optics-protocols-satellite-ocean-colour-sensor-validation/> are the official protocols for the PACE mission.
 - Appropriate references for *in situ* and airborne measurement protocols of aerosol and cloud properties are posted on the PACE website.
- February 2021: Release of ROSES 2021 (TBC) containing solicitation for the PVST. Response due date TBD.
- [TBD]: Responses to ROSES 2021 (TBC) PVST solicitation are due.
- NLT December 2022: Selected PVST Teams begin work.

PVST Teams will communicate with Program Science, Project Science, and SDS within 1-2 months of the start date of the award to review their plans for collection and analysis of field measurements.

The PVST members selected to participate in the PACE Field Validation Mission (directed airborne-shipborne field campaign) will interact with Project Science, Program Science, and SDS as required to prepare for the Field Validation Mission.

PVST Teams may conduct pre-launch field measurement activities to refine their methods [TBD].

- PACE Launch Date (**subject to change**):
 - Project Readiness Date: nominally December 15, 2022
 - Launch Readiness Date: nominally March 31, 2023
- PACE Commissioning: Launch + 2 months
- PACE Operations: 3 years after Launch + 2 months commissioning
- Commencement post-launch validation efforts: Launch + 2 months commissioning
- Duration of post-launch validation efforts: 36 months of science operations

PACE Field Validation Mission commences within 2 months of launch. PVST Teams commence their efforts to collect field measurements for validation of required and advanced PACE science data products after commissioning of the PACE observatory. Field data submissions to SDS (i.e., SeaBASS) commence shortly after measurement collections begin and are completed within 6 months of collection to enable the validation of required PACE data products within 12 months of commissioning.

SDS in coordination with Project Science quality controls the field data submissions and supports the validation matchup analysis for PACE science data products. SDS submits quality controlled field data to the OB.DAAC for archiving.

PVST efforts to collect field measurements for validation of PACE data products concludes after 36 months of PACE Science Operations.

2.5 Elements of a Validation Program

To enable post-launch validation of PACE science data products, HQ PACE Science will assemble a PACE Validation Science Team (PVST). The goal of the PVST will be to collect field measurements with sufficient quality, range of environmental conditions (e.g., aerosol properties, wind speed and direction, solar zenith angles, etc. for ocean color products), dynamic range, and geographic distribution to enable validation of PACE science data products. While the priority of the PACE Validation Program is to validate the required data products, the PVST shall also collect field measurements to validate the advanced science data products where possible. The field measurements necessary for validation of required and advanced science data products are provided in Table 5. A schematic of the organization of the PACE Validation Program interfaces and data flow is provided in Figure 1.

Several elements are essential to enable a successful PACE Validation Program (e.g., McClain et al., 2002).

- a) First and foremost is a formal PACE Validation Science Team dedicated to collecting validation-quality field measurements. In contrast to the PACE Science and Applications Team (SAT), the PVST will not be conducting formal scientific investigations, i.e., addressing particular science research objectives or hypothesis testing.
- b) The PVST shall adhere to scientific community accepted field measurement protocols and meet the required measurement uncertainties. Specifically for ocean field measurements, the relevant protocols are the International Ocean Colour Coordinating Group (IOCCG) Ocean Optics and Biogeochemistry Protocols for Satellite Ocean Colour Sensor Validation (<http://ioccg.org/what-we-do/ioccg-publications/ocean-optics-protocols-satellite-ocean-colour-sensor-validation/>) or other protocols should the IOCCG protocols not address the measurement of interest.
- c) Field instrument calibration capabilities or facilities traceable to NIST, or other national metrology institution.
- d) Field instrumentation used to acquire validation measurements should, ideally, be fully characterized with traceability to NIST or other national metrology institution.
- e) A central facility, where appropriate, for laboratory analysis of field samples to meet required uncertainties. The most relevant example is the NASA GSFC field support lab tasked to quantify chlorophyll-a concentration and other phytoplankton pigments by high-performance liquid chromatography (HPLC). A centralized laboratory can provide a cost-effective mechanism for providing consistently high-quality data, if the facility is dedicated to excellence, maintains rigorous quality assurance and control procedures as part of a well-

documented quality assurance plan, and adheres to performance metrics to minimize uncertainties.

- f) Field data archive (SeaBASS, AERONET, or other) as repository of field measurements including airborne campaign data.
- g) Dedicated team(s) performing matchup validation analysis of available field measurements with PACE-derived science data products. For PACE, Project Science in coordination with SDS will accomplish the formal science data product validation for the mission.
- h) Utilize all available resources, which meet data quality requirements, including existing infrastructure and datasets supported by NASA (AERONET, AERONET-OC, etc.) and other agencies (Bio-Argo, MOBY, time-series stations such as BATS and HOT).
- i) Enables a broad range of approaches for collecting sufficient quantities of validation-quality field measurements for validation of PACE science data products within 12 months of commissioning and will continue thereafter through mission lifetime (Table 6).
- j) The PACE Science and Applications Team members supported to collect field measurements to accomplish science objectives including algorithm development shall adhere to the same measurement protocols and calibration traceability as the PVST.

Table 5. Field measurements necessary for validation of PACE ocean, aerosol, and cloud data products. Appropriate measurement protocols will be specified in each Algorithm Theoretical Basis Document (ATBD).

<i>Ocean Properties</i>	Range	Measurement Uncertainty
Ocean field measurements for required data products		
Remote sensing reflectances centered on (± 2.5 nm) 350, 360, and 385 nm (15 nm bandwidth)	0.0015 – 0.020 sr ⁻¹	<4%
Remote sensing reflectances centered on (± 2.5 nm) 412, 425, 443, 460, 475, 490, 510, 532, 555, and 583 (15 nm bandwidth)	0.0008 – 0.033 sr ⁻¹	<4%
Remote sensing reflectances centered on (± 2.5 nm) 617, 640, 655, 665, 678, and 710 (15 nm bandwidth, except for 10 nm bandwidth for 665 and 678 nm)	0.000 – 0.012 sr ⁻¹	<5%
Advanced/goal ocean measurements		
Remote sensing reflectances 350-400 nm (5 nm bandwidth)	0.0015 – 0.020 sr ⁻¹	<4%
Remote sensing reflectances 400-600 nm (5 nm bandwidth)	0.0008 – 0.033 sr ⁻¹	<4%
Remote sensing reflectances 600-720 nm (5 nm bandwidth)	0.000 – 0.012 sr ⁻¹	<5%
Total absorption coefficient (350-750 nm) ¹	0.000 – 2.000 m ⁻¹	TBD
Particulate absorption coefficient (350-750 nm) ¹	0.003-1.5 m ⁻¹	TBD
Phytoplankton absorption coefficient (350-750 nm) ¹	0.003-1.2 m ⁻¹	TBD
Non-algal particle absorption coefficient (350-750 nm) ¹	0.0004 – 0.6 m ⁻¹	TBD
Non-algal particle plus dissolved organic matter absorption coefficient (350-750 nm) ¹	0.002-1.5 m ⁻¹	TBD
Particulate backscatter coefficient (350-750 nm) ¹	0.0001-0.1 m ⁻¹	TBD
Total backscatter coefficient (350-750 nm) ¹	⁶ 0.0005-0.1 m ⁻¹	TBD
Chlorophyll-a concentration ¹	0 – 330.3 mg m ⁻³	$\leq 5\%$ ¹²
Diffuse attenuation coefficients (350-750 nm) ¹	TBD	TBD
Particulate organic carbon concentration ¹	⁷ 0 – 2000 mg m ⁻³	$\leq 14\%$ ¹²
Dissolved organic carbon concentration ¹	⁶ 35 – 1000 mmol m ⁻³	<5%

Particulate inorganic carbon concentration ¹	⁸ 0.001 – 10 mmol m ⁻³	Awaiting protocols - TBD
Vertical carbon flux	⁹ 0 – 500 mg C m ⁻² d ⁻¹	TBD
HPLC phytoplankton pigments concentration ¹		
Primary pigments	¹⁰ 0 – 330.3 mg m ⁻³	≤10% ¹²
Photosynthetic pigments	¹⁰ 0 – 530.3 mg m ⁻³	≤6% ¹²
Photoprotective Pigments	¹⁰ 0 – 71.9 mg m ⁻³	≤11 ¹²
Individual photosynthetic pigments	¹⁰ 0 – 330.3 mg m ⁻³	5.4-22.9% ¹²
Individual photoprotective pigments	¹⁰ 0 to 49.2 mg m ⁻³	8.5-35.3% ¹²
Individual primary, secondary, and tertiary pigments (excl. chl-a)	¹⁰ 0 – 137.3 mg m ⁻³	6-67% ¹²
Phytoplankton phycobilin pigments concentration ¹	TBD	Awaiting protocols - TBD
Phytoplankton abundances and community composition to genus/species level ¹	TBD	Awaiting protocols - TBD
Net Primary Production ²	⁹ 0 – 1500 mg C m ⁻³ d ⁻¹	Updates to protocols underway
Colored dissolved organic matter absorption (350-750 nm) ¹		<5%
Photosynthetically available radiation (PAR) (400-700 nm)	0 – 70 mol quanta m ⁻² d ⁻¹	TBD
Fast repetition rate fluorometry (FRRF) - phytoplankton physiology (quantum efficiency, rate of electron transport through photosystem II, iron stress, etc.) ¹	TBD	Awaiting protocols - TBD
Phytoplankton carbon (C _{phyto}) ¹	TBD	Awaiting protocols - TBD
Phytoplankton growth rate ¹	¹¹ 0.01 – 3 day ⁻¹	Awaiting protocols - TBD
Fluorescence quantum yield ¹	TBD	Awaiting protocols - TBD
Surface ocean wind vectors	TBD	TBD
Water-leaving reflectances	TBD	TBD
Particle size distribution ¹	TBD	TBD
Bulk refractive index ¹	TBD	TBD
Scattering coefficient ¹	TBD	TBD
Ratio of attenuation to absorption ¹	TBD	TBD
Water temperature ³	TBD	TBD
Salinity ³	TBD	TBD
Density ³	TBD	TBD
Aerosol properties	Range	Uncertainty
Aerosol field measurements for required data products		
Total aerosol optical depth at 380 nm	0.0 to 5	0.01 to 0.02
Total aerosol optical depth at 440, 500, 550 and 675 nm over land	0.0 to 5	0.01 to 0.02
Total aerosol optical depth at 440, 500, 550 and 675 nm over oceans	0.0 to 5	0.01 to 0.02
Fraction of visible aerosol optical depth from fine mode aerosols over oceans at 550 nm	0.0 to 1	0.1 to 0.15
Aerosol field measurements for advanced data products		
Aerosol size distribution	0.01-20 μm	TBD
Aerosol absorption coefficient (spectral – if available)	0.1-100 Mm ⁻¹	TBD
Aerosol scattering coefficient (spectral)	1-1000 Mm ⁻¹	TBD
Aerosol (polarized) phase function ⁴	TBD	TBD
Cloud properties	Range	Uncertainty
Cloud field measurements for required data products		

Cloud layer detection for optical depth < 0.3	Binary yes/no	n/a
Cloud top pressure of opaque (optical depth > 3) clouds	1000-50 hPa	< 50 hPa
Optical thickness of liquid clouds	2-150	< 20%
Optical thickness of ice clouds	2-150	< 20%
Effective radius of liquid clouds	2-100 μm	< 20%
Effective radius of ice clouds	2-100 μm	< 20%
Water path of liquid clouds	0-500 g m^{-2}	< 30%
Water path of ice clouds	0-500 g m^{-2}	<30%
Cloud field measurements for advanced data products		
Effective variance of liquid clouds	0.01-0.5	
Ice crystal (polarized) phase function		
Ice crystal aspect ratio/shape ⁵		

¹ Vertical profile measurements sufficient to derive optically-weighted profiles within the first optical ocean depth detectable from OCI.

² Measurements sufficient to derive vertically-integrated values within the ocean's euphotic depth.

³ Vertical profile measurements as necessary data for measurement corrections and metadata.

⁴ Used to estimate microphysical properties

⁵ Used to determine crystal roughness

⁶ PACE Science Definition Team, 2018

⁷ Stramski et al., 2008

⁸ Balch et al., 2018

⁹ Siegel et al., 2014

¹⁰ C. Thomas, personal communication

¹¹ Laws, 2013

¹² Hooker et al., 2012

2.5.1 Field Measurement Protocol Development for Satellite Ocean Color Data Products

The importance of community-vetted field measurement protocols for validation of ocean color satellite data products extends to the SIMBIOS project. With support from the PACE Science Data Segment, the GSFC field support team continues to collaborate with the international scientific community of experts to update the prior SIMBIOS-era NASA Ocean Optics Protocols for field measurements (Mueller et al. 2003) and establish new field measurement protocols for the purposes of validating ocean color satellite data products. The process nominally entails the following steps:

- a) A team of experts is assembled at a workshop to review the state-of-the-art on the particular field measurement approaches and instrumentation.
- b) A protocol outline is developed and leads for each section are identified.
- c) Reporting on protocol document development occurs at appropriate scientific conferences and meetings. Open community workshops may be held in association with conferences or meetings.
- d) A complete protocol document draft is posted on the IOCCG website for a minimum 60-day community feedback period; this is referred to as the "community peer review".
- e) In parallel with the "community peer review", subject matter experts are invited to serve as Associate Editorial Peer Reviewers (AEPR) and asked to provide their own reviews of the protocols.
- f) Once the community and AEPR peer reviews are submitted, the protocol authors revise the protocol document accordingly and forward the revised protocol along with a response letter to the AEPRs for their consideration to determine whether all appropriate peer review comments are adequately addressed.

- g) After AEPRs approve the final version of the technical material, the protocol document is formatted and copy edited.
- h) IOCCG generates cover pages for the protocols and obtains a Digital Object Identifier (DOI) from Ocean Best Practices (<https://www.oceanbestpractices.net>), which provides a permanent document repository for the protocol documents and is maintained by the International Oceanographic Data and Information Exchange (IODE) of the Intergovernmental Oceanographic Commission (IOC) of United Nations Educational, Scientific and Cultural Organization (UNESCO).
- i) IOCCG produces the final protocol document as a pdf and is publicly accessible on the IOCCG website, PACE project website, and Ocean Best Practices.

These protocol documents will be amended periodically with advances in scientific knowledge and instrumentation.

For cloud and aerosol products, the development and description of these measurement protocols may exist externally to IOCCG. For example, the measurement protocol and other documentation for MAN and AERONET exist in publications such as Smirnov et al. (2009) and Giles et al. (2019), respectively, and AERONET website hosted documents such as: https://aeronet.gsfc.nasa.gov/new_web/cruises/MAN_Instructions_and_Protocol.pdf. The SVOB and SDS will identify and provide references to these documents as appropriate.

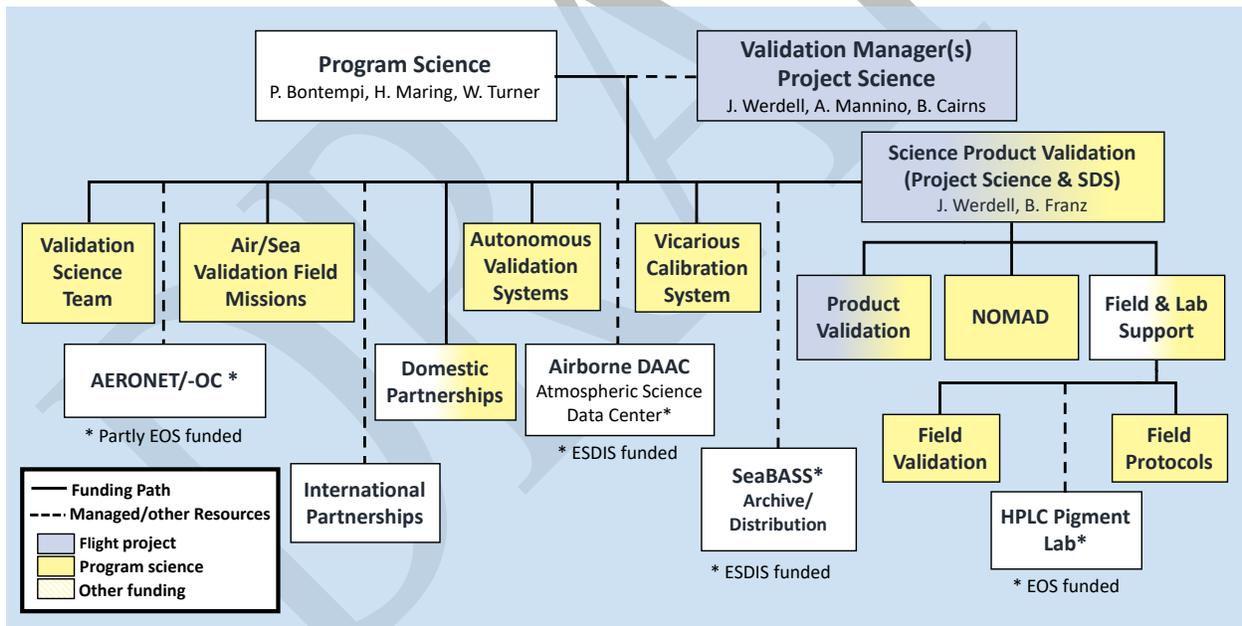


Figure 2. PACE validation program organization and possible validation elements.

2.5.2 Potential Sources of *In Situ* Measurements

Multiple sources of field data will be implemented for validation of PACE science data products (Fig. 2). PVST and other PACE supported activities will provide field validation data through a directed Field Mission and various other approaches as indicated in Table 6. In addition,

existing or planned activities external to PACE are expected to produce field data through the PACE mission lifetime that can be applied for validation of PACE science data products (Table 6). For example, external activities include the well-known AERONET and AERONET-OC projects supported by NASA and other agencies.

Table 6. Potential sources of field measurements for validation of PACE science data products.

	Ocean color	Aerosols	Clouds
Existing infrastructure	AERONET-OC	AERONET	AERONET cloud mode
		MAN	Satellite-to-satellite (VIIRS, GOES, etc.)
External resources	WaterHyperNet	SKYNET; other Sun Photometer networks	Ground-based radar/ceilometer, MWR, MFRSR (ARM, Cloudnet)
	FRM4SOC & non-PACE vicarious calibration sites		Satellite-to-satellite (EarthCARE, Metop-SG IASI-NG/3MI, etc.)
	Data from other agencies	Data from other agencies	Data from other agencies
Possible PACE supported validation activities	Aircraft/Oceanographic validation field mission	Aircraft/Oceanographic validation field mission	Aircraft/Oceanographic validation field mission
	Repeatable field outings		
	Instrumented validation super site (OC & aerosols)	Instrumented validation super site (OC & aerosols)	
	Fleet of small autonomous vehicles		
	PACE-enhanced AERONET-OC sites	PACE-enhanced AERONET/-OC sites	
	PACE vicarious calibration site		
	Field campaigns of opportunity	Field campaigns of opportunity	Field campaigns of opportunity

2.5.3 Elements for the Validation of Multi-Angle Polarimetry

The validation of the multi-angle polarimeter observations has two facets. One is the validation of the polarized radiance data itself and the second is the validation of the aerosol, cloud, and ocean data products derived from the observed polarized radiances. These validation activities will necessarily make use of both the program of record (PoR) and ideally an airborne field campaign focused on validation of PACE atmospheric products.

Validation of radiance and polarization state for the PACE polarimeters

One approach is to use sites with well characterized surfaces and atmospheres (for example the DoE ARM sites and AERONET sites) to forward simulate TOA radiance and polarization in an

approach similar to the vicarious calibration of OCI. The primary limitation of such an approach is that the surface polarization of the available existing sites over land is not adequately characterized. An airborne campaign could include such measurements at low altitude as one part of a PACE atmosphere validation campaign if that is deemed appropriate by the PVST. Otherwise, this approach would of necessity focus on AERONET-OC sites.

The second approach is to use high altitude aircraft flights to intercalibrate the PACE polarimeters against a reference measurement, such as that provided by the Research Scanning Polarimeter (RSP) and/or airborne versions of the two PACE polarimeters. An example of such an approach for a radiometer is McCorkel et al. (2016). Again this could be included as one element of a more general airborne validation campaign for PACE.

Validation of PACE polarimeter data products

Aerosol products: Most products can be validated either directly against AERONET spectral optical depths, or against the higher level AERONET derived products, such as the size distributions, complex refractive indices and single scattering albedos. However, there are significant uncertainties in the complex refractive indices reported by AERONET, and the evaluation and reporting of those uncertainties is the subject of ongoing work (of note is the recent publication Giles et al., 2019). The validation of aerosol vertical layer height products requires a lidar system, either on orbit (e.g., EarthCARE, ICESat-2) or a surface network (e.g., MPLnet, EARLINET). As part of any PACE airborne validation campaign it would be highly desirable to include *in situ* measurements of aerosol size distribution, composition, and absorption over an AERONET site (or sites) to validate the PACE products and understand any limitations in using the AERONET products for validation, along with an airborne lidar.

Cloud products: Many of the PACE polarimeter cloud products can be validated against observations from the ARM sites that include a mid-latitude continental site, a high latitude site, and a site characterized by marine stratocumulus clouds. Validation of some products, such as effective variance, ice particle aspect ratio/roughness and also a rigorous evaluation of cloud particle effective radius would require *in situ* airborne observations carefully coordinated with PACE mission overflights of representative cloud systems (e.g., continental convection, marine stratocumulus off the California coast, post-frontal clouds).

Ocean products: Approaches to validate PACE multi-angle polarimeter ocean data products are generally identical to validating OCI data products. One important consideration will be differences in the pixel dimensions of the satellite data product and the corresponding field measurement.

2.6 Attributes of Appropriate Validation Sites

2.6.1 Ocean Data Products

While it is important to validate PACE data products across a broad range of geographic regions, data product dynamic range and environmental conditions, certain constraints must be considered in the selection of validation sites to provide high-quality validation matchup opportunities. Field validation sites shall either be homogenous across time and space scales relevant for validation of PACE data products (e.g., 3x3, 5x5 or greater science pixel array and

within ± 15 min to ± 3 hours of PACE overflight event) or sufficiently characterized such that the variability in time and space scales of atmospheric and ocean properties are known and within the required PACE validation uncertainty. Bright target effects such as land- or ice-adjacency effects should not compromise the quality of the PACE data products that are being validated. Therefore, measurements for validation of PACE data products shall be collected a minimum of one and ideally three or more science pixels from the shore or ice. Similarly, validation measurements at ocean color validation sites should not be affected by clouds, either directly over the site or from cloud shadows. Bottom reflectance should be insignificant or adequately characterized so that such effects can be taken into account in the validation analysis.

2.6.2 Aerosol Data Products

The validation of PACE aerosol products needs to take place over a range of spatial locations that cover the major aerosol types, as the shape and composition of different aerosols types can impact the retrieved products in different ways. The existing AERONET sites include locations that sample most aerosol types, although a 13:00 local crossing time means that the availability of the higher level AERONET products that use almucantar scans will be quite limited. Recently-released AERONET ‘hybrid’ scan products aim to narrow this gap by providing similar data quality throughout the day. At the time of writing, however, these have not yet been used widely.

Sites that have low surface heterogeneity are preferred because of the impacts that adjacency effects can have on retrievals. Since both coastal and land sites will be used for validation, measures of surface heterogeneity will need to be documented for each AERONET site that is used for validation.

AERONET and its sub-components AERONET-OC and MAN are sufficient to validate required OCI aerosol products (Table 2), as aerosol optical depth is the direct observable of sun photometers, and the fine size mode fraction can be determined from the spectral slope of aerosol optical depth (O’Neill et al., 2003). Validation of advanced OCI, SPEXone and HARP2 aerosol products (Tables 3 and 4) requires retrievals from sky scans (Dubovik et al., 2000), which are available to AERONET and AERONET-OC, but not MAN, and only under conditions with sufficient aerosol loads. This means that other resources are necessary to validate aerosol microphysical properties in the ocean away from AERONET-OC sites, or for cases with low aerosol optical depth. We should also note that AERONET-OC and MAN instruments do not have a channel at 380nm (standard AERONET instruments frequently do), so validation of this optical depth may require interpolation or extrapolation from other spectral channels, or again use of other resources.

2.6.3 Cloud Data Products

The validation of PACE cloud products needs to take place over a range of spatial locations that cover the major cloud system types. The ARM surface sites provide observations of mid-latitude continental, high latitude and stratocumulus cloud regimes at high temporal frequency such that PACE overpasses can be closely matched in space and time. For other cloud regimes the cloud products will be evaluated against other satellite sensors (e.g., JPSS VIIRS/CrIS, Metop-SG IASI-NG/3MI) rather than being formally validated against reference measurements.

2.7 Validation Analysis

PACE Project Science with support from the SDS validation analysis team will perform the formal validation match-up analyses for the PACE mission. Nevertheless, PACE Science and Applications Team members may choose to perform their own validation analyses to evaluate the performance of existing and experimental data product algorithms for the purposes of their particular scientific investigation. The approaches and tools for conducting the validation analysis of PACE science data products will evolve over time.

2.7.1 Ocean Data Products

The PACE validation analysis refers to the analytical evaluation of the field and satellite data match-ups, i.e., the derived satellite data products compared against the *in situ* validation measurements that correspond to the satellite sensor observations in time and space as summarized in the previous section and discussed in detail in Bailey and Werdell (2006). The validation analysis shall implement community-accepted criteria. Current examples of validation analysis criteria include the following:

- Applied to level-2 science data products (unmapped/native resolution for OCI)
- Requires well-defined metrics for evaluation of validation match-up analysis (e.g., Seegers et al., 2018).
- Adheres to documented and community accepted protocols (e.g., Bailey and Werdell, 2006), which entail exclusion of satellite pixels that do not pass quality flagging criteria, exclusion of satellite data within validation site pixel array that exceed filtering criteria, exclude satellite observations from extreme sensor and solar zenith angles, and demonstrate low variability among filtered pixel array values.

The SeaBASS team at GSFC has developed software tools to facilitate validation analysis of ocean color satellite data products from several instruments (SeaWiFS, MODIS, MERIS, VIIRS, etc.) with the field measurements submitted to SeaBASS by the scientific community. These tools shall be further optimized for PACE data products by the PACE SDS validation analysis team.

2.7.2 Aerosol Data Products

The validation of OCI spectral optical depth products will use the AERONET direct sun observations with a typical temporal frequency being every 10 minutes. The network consists of hundreds of stations, located globally, across all continents and in a wide variety of aerosol, meteorological, and surface type conditions (Giles et al., 2019). The configuration of the spectral bands varies, but typically is centered at 0.34, 0.38, 0.44, 0.50, 0.67, 0.87, and 1.02 μm allowing the OCI spectral optical depths to be directly compared by using a quadratic log–log fit (Eck et al., 1999) to interpolate the AERONET AODs to the OCI spectral band centers. Requirements on spatial and temporal matching, depending on the resolution of the product being validated, have been reported in the literature (Remer et al., 2013; Munchak et al., 2013; Virtanen et al., 2018) as have requirements on quality flags and the number of successful retrievals within a pixel level product (Levy et al., 2010). Essentially the same approach can and will be applied to data collected on MAN cruises (Smirnov et al., 2009) as the largely open-ocean complement to AERONET sites.

2.7.3 Cloud Data Products

Validation of cloud products against surface observations is usually focused on horizontally extensive stratus and cirrus clouds. In part, this is because horizontally uniform clouds reduce difficulties (variability) associated with trying to match the nearly instantaneous and typically lower-resolution satellite datasets with the time–height data produced by surface based nadir-pointing radar and lidar systems (e.g., Mace et al., 2005; Dong et al., 2008; Marchand, 2016). In any case, the impacts of variability on cloud products such as effective radius are well documented (Zhang and Platnick, 2011; Painemal et al., 2013; Cho et al. 2015) and screening for heterogeneity and precipitation will therefore be an important aspect of cloud data product validation. As noted above, more careful validation of effective radius products, given the different vertical weightings associated with different OCI spectral bands and with polarimetric observations, will require *in situ* cloud probe measurements.

2.8 Field Campaign Recommendations

Field campaigns utilizing airborne, (fixed) surface, and shipborne measurements can serve several important objectives of the PACE Validation Plan. For our purposes, we define a field campaign as any short term deployment of assets with a focused goal or set of goals. These goals may be PACE validation, or may not, but the field campaign can be useful for validation purposes regardless. Successful validation with field campaign observations can be performed only if a threshold set of measurement types, operating conditions, analysis techniques, and other provisions are met. In this section, the following text describes aspects of a field campaign’s design that should be taken into consideration in order to meaningfully contribute to validation. A more detailed description of these requirements, and how the measurements from such a field campaign would be incorporated into a validation system, will be described in a future document, tentatively titled “Planning for PACE relevant field campaigns.”

Direct validation refers to the validation via direct comparison of a measurement to satellite products listed in Tables 1-4. Specific types of measurements that can directly validate satellite products are in Table 5, while some examples of sources of such data are in Table 6. For this type of validation to be successful, the following conditions should be met:

- a measurement must be relevant to the mission, meaning that it is one of the required or advanced satellite data products,
- measurement uncertainty must be equal to or less than that required of the satellite product, either on an individual basis or in aggregate,
- established and transparent measurement protocols must exist, including:
 - standardized data collection techniques,
 - standardized data processing, screening and labeling,
 - calibration traceability, and
 - assessment of measurement uncertainty,
- observation conditions must be appropriate for comparison:
 - validation data must be collected within defined temporal and spatial limits of satellite observation appropriate for each particular product,

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- scene conditions must be appropriate for successful validation measurement collection,
 - scene conditions must be appropriate for successful satellite data collection,
 - the impact of spatial and temporal scale differences between validation measurement and satellite data are considered,
 - validation measurements must be made concurrently with other measurements relevant to satellite product retrieval, validation measurement generation, and analysis of validation results,
 - a sufficient quantity of validation measurements must be made, and these should span a significant range of potential conditions, and
 - validation analysis must use statistically appropriate techniques.

Because of the large number of satellite data products, a useful technique to track validation capability is to create a **Validation Traceability Matrix (VTM)**. Similar to a Science Traceability Matrix, a VTM instead starts from the satellite data products to validate, and flows through the measurements required to validate satellite data and the requirements of such measurements. The abovementioned list can serve as a guide for the creation of a VTM.

Direct validation can obviously only be performed following PACE commissioning. **Proxy validation** can be a useful means to test measurement techniques and algorithms prior to launch. Such validation requires an (airborne) PACE instrument proxy, that can observe a scene in a manner similar to that of PACE itself. Satellite product retrieval algorithms and data management can be tested with proxy data, which is compared to direct validation measurements as described above. Additional constraints must also be levied on such validation, including confirmation that

- proxy measurement conditions are similar to that of the orbital data, or at least accounted for in product generation,
- retrieved proxy products are generated in a similar manner to that of orbital data,
- proxy direct observations (i.e. radiances) are validated and confirmed prior to their use in a retrieval algorithm, and measurement uncertainties are propagated through the retrieval algorithm, and
- the impact of temporal and spatial scale differences between proxy and satellite retrievals are considered.

Because of the scale differences noted above, proxy validation can also be useful after launch. For PACE, several airborne instruments exist that can act as proxies. An example of a field campaign that met some of the requirements for direct and proxy validation was the Aerosol Characterization from Polarimeter and Lidar (ACEPOL) field campaign (Knobelspiesse et al., 2020, <https://www-air.larc.nasa.gov/missions/acepol/index.html>), which deployed airborne prototypes of HARP2 and SPEXone (among other instruments) on the ER-2. PACE polarimeter proxy validation using data from this campaign is underway (e.g. Fu et al., 2019).

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4 APPENDIX A

4.1 Abbreviations and Acronyms

3MI	Multi-Viewing Multi-Channel Multi-Polarisation Imaging instrument
ACEPOL	Aerosol Characterization from Polarimeter and Lidar
AEPR	Associate Editorial Peer Reviewer
AERONET	Aerosol Robotic Network
AERONET-OC	Aerosol Robotic Network Ocean Color
AOD	Aerosol Optical Depth
ARM	Atmospheric Radiation Measurement
ATBD	Algorithm Theoretical Basis Document
BATS	Bermuda Atlantic Time Series
Bio-Argo	Biogeochemical Argo
CrIS	Cross-track Infrared Sounder
CZCS	Coastal Zone Color Scanner
DAAC	Distributed Active Archive Center
DoE	Department of Energy
DOI	Digital Object Identifier
DTC	Design-to-Cost
EARLINET	European Aerosol Research Lidar Network
EarthCARE	Earth Clouds, Aerosols and Radiation Explorer
ENVISAT	Environmental Satellite
EOSDIS	Earth Observing System Data and Information System
ER-2	NASA high-altitude Earth resources aircraft
ESA	European Space Agency
ESDIS	Earth Sciences Data and Information System
ESDS	Earth Science Data Systems
ESD	Earth Science Division
ESM	Earth Systematic Missions
ESMO	Earth Science Mission Operations (GSFC)
FDF	Flight Dynamics Facility
FOT	Flight Operations Team
FRM4SOC	Fiducial Reference Measurements for Satellite Ocean Colour
FRRF	Fast Repetition Rate Fluorometry
GOES	Geostationary Operational Environmental Satellite
GS	Ground Segment
GSFC	Goddard Space Flight Center
HARP2	Hyper-Angular Rainbow Polarimeter 2
HPLC	High Performance Liquid Chromatography
HQ	Headquarters
HOT	Hawaii Ocean Time Series
HSS	Hyper-spectral scanning radiometer
IASI-NG	Infrared Atmospheric Sounding Interferometer–New Generation

ICESat-2	Ice, Cloud and land Elevation Satellite
IOC	Intergovernmental Oceanographic Commission
IOCCG	International Ocean Colour Coordinating Group
IODE	International Oceanographic Data and Information Exchange
ITAR	International Trade in Arms Regulation
JPSS	Joint Polar Satellite System
KSC	Kennedy Space Center
LS	Launch Segment
MAN	Maritime Aerosol Network
MERIS	Medium Resolution Imaging Spectrometer
Metop-SG	EUMETSAT atmospheric sounding and imaging mission
MISR	Multi-angle Imaging SpectroRadiometer
MOBY	Marine Optical Buoy
MOC	Mission Operations Center
MODIS	Moderate Resolution Imaging Spectroradiometer
MFRSR	Multi-Filter Rotating Shadowband Radiometer
MPLnet	NASA Micro-Pulse Lidar Network
MRD	Mission Requirements Document
MWR	Microwave Radiometer
NAAMES	North Atlantic Aerosols and Marine Ecosystems Study
NASA	National Aeronautics and Space Administration
NEN	Near Earth Network
NISN	NASA Integrated Services Network
NIST	National Institute of Standards and Technology
NOAA	National Oceanic and Atmospheric Administration
NOMAD	NASA bio-Optical Marine Algorithm Dataset
NPR	NASA Procedural Requirement
OB.DAAC	Ocean Biology DAAC
OBPG	Ocean Biology Processing Group
OCI	Ocean Color Instrument
ORACLES	ObseRvations of Aerosols above CLouds and their intEractionS
PACE	Plankton, Aerosol, Cloud, ocean Ecosystem
PAR	Photosynthetically Available Radiation
PLRA	PACE Program Level Requirements Agreement
PSRD	PACE Project Science Requirements Document
PVST	PACE Validation Science Team
SAT	PACE Science and Applications Team
SBU	Sensitive But Unclassified
SDS	Science Data Segment
SeaBASS	SeaWiFS Bio-optical Archive and Storage System
SEAC ⁴ RS	Studies of Emissions and Atmospheric Composition, Clouds, and Climate Coupling by Regional Surveys
SeaDAS	SeaWiFS Data Analysis Software
SeaPRISM	SeaWiFS Photometer Revision for Incident Surface Measurement
SeaWiFS	Sea-Viewing Wide Field-of-View Sensor

SIMBIOS	Sensor Intercomparison for Marine Biological and Interdisciplinary Ocean Studies
SIPS	Science-Investigator led Processing System
SKYNET	Ground-based radiation observation network dedicated to aerosol-cloud-solar radiation interaction research
SN	Space Network
SPEXone	Spectro-Polarimeter for Exploration
SS	Space Segment
SVOB	PACE Science Validation Program Operations Board
SWIR	Shortwave Infrared
TBD	To be determined
TBR	To be revised
TBS	To be scheduled
TOA	Top-of-Atmosphere
UNESCO	United Nations Educational, Scientific and Cultural Organization
USGS	United States Geological Survey
VTM	Validation Traceability Matrix
VIIRS	Visible Infrared Imaging Radiometer Suite

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