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PACE Technical Report Series, Volume 8

Editors: Ivona Cetinić, Charles R. McClain, and P. Jeremy Werdell

PACE Science Data Product Selection Plan

Jeremy Werdell, Bryan Franz, Paula Bontempi, Kevin Murphy, Antonio Mannino, Brian Cairns, Sean Bailey, Woody Turner, Jeremy Werdell, and Antonio Mannino

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INTRODUCTION

Introduction to Volume 8: The PACE Science Data Product Selection Plan

The Plankton, Aerosol, Cloud, ocean Ecosystem (PACE; https://pace.gsfc.nasa.gov) mission represents NASA's next great investment in satellite ocean color and the combined study of Earth's ocean-atmosphere system. At its core, PACE builds upon NASA's multi-decadal legacies of the Coastal Zone Color Scanner (1978-1986), Sea-viewing Wide Field-of-view Sensor (SeaWiFS; 1997-2010), Moderate Resolution Imaging Spectroradiometers (MODIS) onboard Terra (1999-present) and Aqua (2002-present), and Visible Infrared Imaging Spectroradiometer (VIIRS) onboard Suomi NPP (2012-present) and NOAA-20 (2017-present). The ongoing, combined climate data record from these instruments changed the way we view our planet and – to this day – offers an unparalleled opportunity to expand our senses into space, compress time, and measure life itself.

This volume presents PACE Project's plan for science data product selection. The PACE observatory includes three science instruments, the combination of which advances far beyond heritage measurement capabilities. The primary Ocean Color Instrument (OCI) consists of two spectrometers that continuously span the ultraviolet to orange and orange to near-infrared spectral regions. Additional detectors will collect measurements at seven discrete shortwave infrared bands, six of which are at similar wavelengths to those on heritage missions to support both atmospheric and ocean color applications. The observatory also includes two small multi-angle polarimeters with spectral ranges that span the visible to near-infrared region. Namely, the Spectro-polarimeter for Planetary Exploration (SPEXone), in development by a Netherlands-based consortium consisting of the Space Research Organization of the Netherlands (SRON) and Airbus Defence and Space Netherlands, and the Hyper Angular Research Polarimeter (HARP2), in development by the Earth and Space Institute at the University of Maryland Baltimore County.

This instrument payload will revolutionize the way we look at our home planet through an increasing range and diversity of possible geophysical data products. The recently assembled PACE Science and Applications Team (SAT; see https://pace.gsfc.nasa.gov) proposed a substantial dynamic range of approaches for possible implementation into NASA standard data processing. The Earth science communities at large also offer a variety of methods for geophysical data product generation that may further maximize PACE science capabilities. In anticipation of an influx of concepts for consideration, the PACE Project developed this Science Data Product Selection Plan. Its purpose is to develop and clearly outline an equitable process for the proposal, implementation, and performance assessment of new and revised PACE science data products. Routine, open, and collaborative interactions with algorithm providers remains, of course, key to the success of this process.

We eagerly await the realization of the revolutionary science that the PACE instrument suite will provide.

P. J. Werdell
PACE Project Scientist
August 2020

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1 INTRODUCTION

1.1 Purpose and Scope

This document describes the flow of and process for the selection and implementation of science data products for the Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) mission. Its scope encompasses threshold/standard mission products and baseline/advanced mission products.

1.2 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 (HARP-2) 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 to shortwave infrared (SWIR) to enable advanced ocean color and heritage cloud and aerosol particle science.
The HARP-2 and SPEXone are secondary instruments on the PACE observatory, acquired outside of GSFC. The HARP-2 is multi-spectral, wide swath (supporting atmospheric correction of OCI) and hyper angular (good for clouds). The SPEXone is narrow swath and hyperspectral, better for characterizing aerosol microphysical properties.

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, HARP-2, 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. 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 of 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/GSFC institutional capabilities 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 and stored 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.

1.3 Applicable and Reference Documentation

1. PACE Program Level Requirements Agreement (PLRA), PACE-SYS-REQ-0007
2. PACE Mission Requirements Document (MRD), PACE-SYS-REQ-0019
3. PACE Project Science Requirements Document (PSRD), PACE-SCI-REQ-0027
4. PACE Science Data Segment Performance Requirements Document (SDSRD), PACE-SDS-REQ-0088
5. PACE Project Science to Science Data Segment Interface Control Document, PACE-SCI-ICD-012
6. PACE Science Data Segment (SDS) to Ocean Biology (OB) Distributed Active Archive Center (DAAC) Interface Control Document, PACE-SCI-ICD-0013
7. Inter-Project Agreement Between the Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) Project and the ESDIS Project for Science Data Archive and Distribution Support, PACE-MGMT-ICD-0054

2 PACE SCIENCE DATA PRODUCT SELECTION

2.1 Overview of PACE Data Products

The PACE mission is required to produce and distribute ocean, atmospheric aerosol, and cloud science data products as described in the PACE Program Level Requirements Agreement. Heritage algorithms from MODIS and VIIRS will initially be adopted for generating these required science data products. This Plan outlines the review and selection process that will be followed to update and/or replace the algorithms and approaches used to produce the standard suite of PACE science data products, or to approve adoption of new data products and algorithms for standard production and distribution.

2.2 Roles in Science Data Product Selection

Several entities work collaboratively to select, implement, evaluate, archive, and distribute science data products. The following describes the core entities.

Contributors

Contributors provide algorithms and approaches, including related documentation, prototype software, and performance metrics, to produce standard and evaluation science data products. Contributors may include the PACE Project Science Team, competitively-selected PACE science team members, and collaborators in the international science and user community.

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. The 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.

Science Operations Board

A Science Operations Board (SOB) provides overall guidance and oversight for the science data selection and classification process described in this Plan. The SOB is responsible for approving changes to the suite of science products produced and associated algorithm approaches employed for operational (routine) production by the SDS and distribution by the NASA-assigned DAAC. For PACE, this SOB will consist of the Project Scientist, Deputy Project Scientist(s), Mission Program Scientist, Deputy Program Scientist(s), SDS Manager, OB.DAAC Manager, and an ESDIS Program representative.

Science Operations Team

The Science Operations Team (SOT) is a working-level subset of the SOB, established to provide a first-level of review for proposed product and algorithm changes. The SOT will work with the Contributor to gather the information necessary for review by the SOB. The SOT has the authority to approve implementation and testing of new products and algorithms for the purpose of establishing resource requirements and verifying operational feasibility. The SOT will also assess if a change is major (e.g., new product or approach) or minor (e.g., refinement of existing algorithm coefficients). For PACE, this SOT will consist of the Project Scientist, SDS Manager, and select members of their teams.

2.3 NASA Data Product Classifications and Maturity Levels

All PACE science data products will be classified as either *standard*, *provisional,* or *test*, following ESDIS/EOSDIS and NASA's Science Mission Directorate (SMD) standards. EOSDIS provides the following classifications for data products:

Standard

A data product produced at a DAAC by a community consensus algorithm for a wide community of users.

> For PACE, standard science data products will be produced by the SDS and delivered to the NASA-assigned DAAC for permanent archival and distribution. PACE standard science data products include all required mission products as described in the PLRA, as well as any additional advanced products selected as standard through the process described in Section 2.5.

Provisional

Product was defined to facilitate data exploration and process studies that do not require rigorous validation. These data are partially validated and improvements are continuing; quality may not be optimal since validation and quality assurance are ongoing.

> For PACE, all standard products will be defined as provisional at-launch, and all new products proposed to become standard products will be defined as provisional at start of production, and they will remain provisional until some level of validation has been performed, and performance, documentation, and science value is deemed sufficient for reclassification as standard products.

Test

Products intended to enable users to gain familiarity with the parameters and the data formats.

> For PACE, Beta products are those that have been implemented by the SDS into production-capable science code, to enable assessment of resource requirements and feasibility for global production.

2.4 Science Data Product Documentation

2.4.1 Approved Product List

The Approved Product List (APL) is the master list of Standard and Provisional products currently recognized by the SOB. For each product, the APL will list:

1. Product name
2. Brief description
3. Link to detailed Product and Algorithm Description Document (PADD)
4. Product maturity (provisional or validated)

In some cases, a product may contain many sub-products (e.g., spectral elements, constituent components, valuable secondary products), which should be detailed in the description, or broken-out as separate products with the same algorithm, as necessary and appropriate to indicate the actual number of individual parameters to be generated.

For PACE, the initial APL will be established by the Project Scientist and approved by the SOB prior to Phase D. The initial APL will be derived from the required mission product list as detailed in the PLRA, plus any additional goal products that are expected to be produced by the SDS at launch. Any further changes to the APL must be reviewed and approved by the SOB (Section 2.5). The APL will be available on-line through the PACE Project website.

2.4.2 Product and Algorithm Description Document

Every standard or provisional product will have an associated Product and Algorithm Description Document, PADD). The PADD will serve the role of the EOS-era Algorithm Theoretical Basis Document (ATBD), as well as the product user's guide and a centralized location for details of implementation and product quality assessment. These PADDs will be living, online documents and provide the following content:

1. Approach and Implementation
   a. Brief description of the product
   b. Description of the algorithm and implementation approach, with references to any existing peer-reviewed literature for additional details
   c. Hyperlinks to key software
2. Assessment of product uncertainties
   a. Approach to estimating uncertainties
   b. Current state of knowledge
3. Assessment of product quality
   a. Validation approach
   b. Table or hyperlink to results

Every product will have an assigned point of contact (POC), which will typically be the algorithm Contributor or the Project Scientist. The product POC will be responsible for maintaining the content of the PADD, while the SDS will support PADD implementation and

delivery to the DAAC, and the DAAC will provide and maintain on-line access for the user community. A draft PADD will be required before SDS will produce a provisional product, and the final PADD will be delivered to the DAAC at the same time as the associated data products. All PADDs will be available on-line from the DAAC website.

2.4.3 Product Change Requests

All product and algorithm changes, either for new products or updates to existing algorithms, will be initiated using the PACE Product Change Request (PCR) form (Appendix A). The PCR form and submission mechanism will be available on-line, as will the list and status of all PCRs currently under consideration.

2.5 Science Data Product Lifecycle

The process for updating, replacing, or re-classifying a PACE science product algorithm, or for introducing an approach to generate a new PACE science data product, is as follows:

1. A Product Change Request (PCR) is submitted.
2. The SOT meets to review the request. If the change is deemed minor but necessary, the SOT initiates the update to the operational software as per the Project Science to SDS ICD. If the change is deemed major, and if the information provided is deemed sufficient, the SOT authorizes implementation and testing by the SDS (*test* product generation), and works with the requester to collect the resource requirements and documentation (PADD), including a preliminary assessment of algorithm performance, as required to enable SOB review. The SOT initiates the SOB review.
3. The SOB reviews the PCR and associated materials, and performs an impact assessment to verify that sufficient computing resources are available to generate the product. Following a positive review, the SOB authorizes the SDS to produce a provisional product for distribution by the DAAC, or to implement a major algorithm change to an existing product at the next reprocessing opportunity. The SOB updates the APL to reflect the change.
4. Periodically (e.g., semi-annually or prior to a major reprocessing), the SOT will initiate SOB review of the APL to assess the maturity classification of all standard and provisional products, determine if any provisional products should be elevated to standard products, and decide if any standard or provisional products or approaches should be discontinued. At this time, the SOB may choose to initiate an additional (external) panel review or community comment period to better gauge scientific consensus.

2.6 Dissemination of information

The PACE Project will maintain the approved product list products on the Project website (https://pace.gsfc.nasa.gov) for the duration of the mission. Pre-launch, this will also include product PADDs and links to preliminary performance and uncertainties assessments. Post-launch, this information will also be transferred to the NASA-assigned DAAC, and it will be expanded to include data product validation activities and results.

Appendix A PACE Product Change Request Form

PACE Science Product Change Request

Title:

Change Type (*new product, algorithm or enhancement*)

Change Description (*e.g., algorithm, code, input data)*:

Scientific Rationale for the Change (*what need does this address, and what is the expected result?)*:

Applicability (*e.g., entire mission data set, specific time range, region or conditions*)

Change Evaluation/Validation Process (*e.g., data sets or time ranges that need to be processed by ADPS, analysis to be performed, any additional data required)*

Documents Affected (*e.g., PADD, software description, format specification*)

List of Attachments (e.g., *source code files, tables)*

Appendix B Abbreviations and Acronyms

[Alphabetize list]

ATBD	Algorithm Theoretical Basis Document
DAAC	Distributed Active Archive Center
ESDIS	Earth Science Data and Information System
GSFC	Goddard Space Flight Center
HARP-2	Hyper-Angular Rainbow Polarimeter 2
ITAR	International Traffic in Arms Regulation
MODIS	Moderate-resolution Imaging Spectroradiometer
OCI	Ocean Color Instrument
PACE	Plankton, Aerosol, Cloud, ocean Ecosystem
PADD	Product Algorithm Description Document
PCR	Product Change Request
SBU	Sensitive But Unclassified
SDS	Science Data Segment
SMD	Science Mission Directorate
SOB	Science Operations Board
SOT	Science Operations Team
SPEXone	Spectro-Polarimeter for Exploration
TBD	To be determined
TBR	To be revised
TBS	To be scheduled
VIIRS	Visible Infrared Imaging Radiometer Suite

Previous Volumes in This Series

Volume 1 *April 2018*	ACE Ocean Working Group recommendations and instrument requirements for an advanced ocean ecology mission
Volume 2 *May 2018*	Pre-Aerosol, Clouds, and ocean Ecosystem (PACE) Mission Science Definition Team Report
Volume 3 *October 2018*	Polarimetry in the PACE mission: Science Team consensus document
Volume 4 *October 2018*	Cloud retrievals in the PACE mission: Science Team consensus document
Volume 5 *December 2018*	Mission Formulation Studies
Volume 6 *December 2018*	Data Product Requirements and Error Budgets
Volume 7 *December 2018*	Ocean Color Instrument (OCI) Concept Design Studies