PACE Science Data Reprocessing Version 3.x

The initial public release of PACE science data products (Version 1) began on 11 April 2024, and provided the science and applications user community with access to the Level-1 data and a limited suite of derived products from the OCI, HARP2, and SPEXone instruments, with the caveat that the data were in a highly preliminary state and should be used with caution. Reprocessing Version 2 was the first full mission reprocessing, and primarily served to incorporate improved calibration knowledge from on-orbit measurements collected by the three PACE instruments. Reprocessing Version 3 includes a further refinement of the calibration for the three instruments, as well as various algorithm refinements, bug fixes, data format improvements, and expanded product suites. For OCI, an additional refinement of the geophysical products at Level-2 and Level-3 was performed in August of 2025, with those derived products tagged as Version 3.1. The 3.1 OCI reprocessing also included a very small change to the Level-1B products to correct for a ghosting artifact in a narrow range of scan pixels and spectral bands, as previously identified in the known issues for Version 3. The Level-1B and 1C products for OCI are still tagged as V3, but the internal version metadata will indicate V3.0.1 after ghosting corrections are applied.

The notes that follow provide an overview of the changes introduced between Version 2 and Version 3, for the Level-1 products of each instrument, and between Version 2 and Version 3.1 for the derived science products currently available. For a comprehensive list of the science data products planned for PACE and the current status of those products and algorithms see the PACE Data Products Table.

PACE Level-1C Grid

Changes from Version 2 to Version 3:

- For all instrument, the Level-1C granules at high latitudes, crossing the day/night terminator, showed significant geometric artifacts and frequent failures. The issue was traced to a software error, which has been fixed in V3. In addition to resolving the high-latitude granules, the correction results in a slight shift in the geographic location of the grid centers for all Level-1C granules by 10s of meters.

OCI Level-1A/B/C Data (Provisional)

Changes from Version 2 to Version 3:

- The OCI absolute calibration coefficients were revised by relying exclusively on the on-orbit solar diffuser calibration (previously: the calibration was prelaunch-based with adjustments derived from the solar diffuser measurements). The update for V3 significantly increases the observed radiances in the UV spectral range, with more modest changes over the full spectral range.
- The OCI temporal gain degradation now takes into account the degradation of the reflectance of the daily solar diffuser, thus improving OCI temporal stability.

- Occasional outliers are seen in OCI dark data, especially in the area of the South Atlantic Anomaly. These outliers can corrupt the background subtraction for a complete scan line, leading to striping in the L1B data. The algorithm to calculate the background subtraction in the L1B code has been improved to remove these outliers end thus remove he striping artifacts. Single pixel outliers in the earth view data may still be present.
- Geolocation accuracy was further improved through use of definitive ephemerides, updated sensor alignments, and improved sensor scan geometry.
- The integrated solar irradiances for each OCI band, as provided in the Level-1B and used to normalize the observed radiance to a reflectance, were updated to use a more appropriate integration approach. This change reduces non-physical spectral variability in the derived reflectance, especially in the UV-blue spectral region.

Updates to Version 3 to Version 3.0.1:

- A correction for ghosting in the observed radiances has been applied, with impact to spectral bands between 650nm and 900nm in a narrow range of scan pixels between 680and 800. Previously, horizontal striping was observed in these bands for scan angles from +3.9deg to +14.6deg (scan pixels 680 to 800). For uniform scenes, the TOA signal usually varies by less than 1% due to this effect, but close to bright sources (such as a coastline) the striping over ocean could be several percent. The striping is usually too small to detect over land or clouds. The likely reason for the striping is spatial and spectral crosstalk impacting half-angle mirror side 2.

Known Issues and Data Characteristics:

- Data in the transition region between the red and blue focal planes, between 590 and 610nm, often shows significant discontinuity. Measurements in this range have much higher uncertainty and should not be used for science algorithms.
- Some SWIR bands show significant signs of apparent band-to-band registration issues. Based on prelaunch measurements, bands 1038nm and 1250nm (Standard Gain), and 1615nm (Standard Gain) with large radiance gradients to neighboring pixels in scan direction are expected to be impacted the most.
- The optical design of the OCI SWIR detector assembly (SDA) causes the bands to view different locations along-scan at a given time, and the data are packetized by time. The bands are pixel-shifted into alignment with the hyperspectral bands. This results in fill pixels at the start or end of the scan, depending on the required pixel shift. The worst case is the 2260 nm band that has 13 fill pixels at the start of the scan. This is a feature of the instrument design.
- Data below 340nm has not been characterized prelaunch as completely and accurately as the data above 340nm. The data below 340nm is only released to facilitate assessment and potential refinement of radiometric accuracy and should not be considered as science quality.

- The blue focal plan bands (310 – 610 nm) are known to have crosstalk that is significant in some bands, particularly in the UV range. The correction for this is still being developed and is planned for Version 4.
- There is an issue with the terrain correction that causes negative height values, primarily along coastlines. This will be corrected in Version 4.

OCI Level-2 & Level-3 Science Data Products

OCI Level-2 products are organized into product suites, with each suite in one file per granule. In some cases, the Level-2 products suites contain a mix of Provisional, Test, and Diagnostic products. The Level-2 products are then binned and mapped into global composites at various temporal (daily, monthly) and spatial resolutions (0.1-deg, 1-deg).

OC_AOP, Ocean Color Apparent Optical Properties:

Provisional Products
- Remote Sensing Reflectance (Rrs)
- Rrs Uncertainties (Rrs_unc)
- Apparent Visible Wavelength (avw)
- Normalized Fluorescence Line Height (nflh)

Diagnostic Products
- Aerosol Optical Thickness (aot)
- Aerosol Angstrom Exponent (angstrom)

Changes from Version 2.0 to Version 3.0:
- The updated Level-1B instrument calibration was applied, and system vicarious calibration (SVC) gains have been derived and applied for the first time. The derived SVC gains for V3 are based on measurements from HyperNAV sites near Mo'rea and Hawaii.
- While OCI was designed to minimize sensitivity to polarization state of the observed radiance, some small residual sensitivity still exists, and this was characterized prelaunch. A correction for this residual sensitivity was implemented for the first time in V3 of the ocean color processing. Note that the correction is discipline-specific, and implemented in Level-2 processing, as it requires modeling of the polarization state of the incoming light.
- Significant improvement was made to the atmospheric gas transmittance algorithm and associated look-up table (LUT) that reduces residual error in the spectral vicinity of strong gas absorption features (H2O, O2, etc.). NO2 corrections were enabled, consistent with heritage MODIS & VIIRS algorithm.
- When the OCI instrument tilt changes, near the subsolar point of the PACE orbit, the sensor passes through extreme glint conditions (direct specular reflection). This results in systematic artifacts in the Rrs retrievals due to error in the atmospheric correction. In

V2, these cases were flagged as high glint but not masked. In V3, the most extreme glint conditions are masked, and no retrieval of Rrs is attempted.

- The subsurface light field model used in the bidirectional reflectance (BRDF) algorithm was previously developed for MERIS, and was defined on the multispectral wavelengths of that sensor. For V3, the BRDF look-up table was regenerated for the hyperspectral wavelengths of OCI, including extension into the UV.
- Rrs products in the 340-345nm and 590 to 610 nm spectral range have been removed, due to artifacts associated with instrument performance in those spectral ranges.
- Rrs retrievals generally increased in the blue spectral range, due to the instrument calibration and addition of NO2 corrections.
- Chlorophyll Fluorescence Line Height (nFLH) has been added to the AOP suite
- AVW has been elevated to Provisional status.

Changes from Version 3.0 to Version 3.1:

- The ghosting correction to the Level-1B instrument calibration was applied. The impact is observable in the retrieved Angstrom exponent (and to lesser extent in AOT and Rrs), as reduced striping artifacts near the center of the OCI swath and southeast of bright sources like coastlines.
- The vicarious calibration (SVC) gains were updated. The largest impact is in wavelengths longward of 650nm, where a mistake in the derivation of the V3.0 gains resulted in a slight over-calibration in the red.
- The absorbing gas corrections were further refined, leading to reduced artifacts near the O2b-band at 680-nm and spectral regions where water vapor absorption is significant.
- The ancillary relative humidity (RH) used in atmospheric correction is now taken from the MERRA2 profile at 925mb pressure, rather than from the 10-meter near-surface values. RH is used to define the size of coarse-mode aerosols and thus to restrict the set of aerosol models to be considered in the atmospheric correction. The change in RH source provides a better estimate of the humidity where the aerosols are found, and generally results in larger aerosol particles that should yield aerosol models (phase functions) more consistent with observations. The impact is to reduce special artifacts in the Rrs retrievals near the backscattering direction (170-180deg scattering angle).
- The glint correction was updated to include spectral dependence on the index of refraction of seawater, which has a significant impact in the shortwave infrared region.
- The Chlorophyll Fluorescence Line Height (nFLH) algorithm was adjusted to minimize impact from absorbing gas artifacts, and generally to better handle low signal levels. The impact is to improve retrievals and minimize negative values in low fluorescence regions.

Changes from Version 3.1 to Version 3.2:

- OCI has low polarization sensitivity, but a small correction was implemented and first applied in V3.0. That implementation did not properly compute the geometry across

scan, and that implementation has now been corrected. This has a very small impact on cross-track and latitudinal variation of Rrs.
- In V3.1 (and prior versions), the bidirectional reflectance (BRDF) correction was not correctly accounting for the change in relative azimuth across the scan. This has been corrected, resulting in a significant improvement in accuracy and cross-track stability of the Rrs retrievals.
- The absorbing gas corrections were further refined …
- The vicarious calibration (SVC) gains were updated to account for impact of small changes in the atmospheric correction algorithm, and to incorporate additional OCI observational match-ups with measurements from the HyperNAV SVC sites.
- Level-2 ocean color retrievals are flagged for presence of coccolithophores, as the derived bio-geochemical properties are likely biased in these highly scattering conditionsAll ocean color Level-3 products in V3.1 (and earlier) were masked for coccolithophores. In V3.2, that masking has been disabled for the AOP products, as it was determined that the Rrs retrievals in the presence of moderate coccolithophore concentrations are valid. At high concentrations, the AOP products can still be masked for atmospheric correction failure.

Known Issues:
- Performance of Rrs retrieval in the UV (below 400nm) has not been validated and is likely to contain significant biases and erroneous variability.
- Corrections for absorbing gases continue to improve, but Rrs variability, especially in the red, is still likely to contain residual artifacts from water vapor and oxygen absorption.
- The current processing extends to higher view zenith angles than the heritage sensors. The atmospheric correction becomes increasingly difficult at these extreme geometries, and erroneously elevated reflectance has been observed in red wavelengths near scan edge. These data are flagged in Level-2 and masked in Level-3 (above 60-degrees).
- Chlorophyll Fluorescence Line Height (nFLH) is displaying impacts of the erroneously elevated reflectances at the scan edge, and in extreme cases, is also impacted by the O2 b-band absorption artifacts in 680nm region.

OC_IOP (Ocean Inherent Optical Properties):

Provisional Products
- Total absorption coefficient (a)
- Total backscatter coefficient (bb)
- Phytoplankton absorption coefficient (aph)
- Phytoplankton absorption coefficient standard uncertainty (aph_unc)
- Non-algal particle plus chromophoric dissolved organic matter absorption coefficient (adg)
- Non-algal particle plus chromophoric dissolved organic matter absorption coefficient standard uncertainty (adg_unc)

- Particle backscattering coefficient (bbp)
- Particle backscattering coefficient standard uncertainty (bbp_unc)
- Spectral diffuse attenuation coefficient (Kd)

Diagnostic Products
- Mean residual of model fit (rrsdiff)

Changes from Version 2.0 to 3.0:
- Products are derived from Rrs. See OC_AOP: Rrs changes and known issues. Impact is improved retrieval performance, increased coverage due to reduced negative Rrs retrievals.

Changes from Version 3.0 to 3.1:
- Spectral range of output products is now restricted to 400-720nm. Previous version included 350-400nm, where IOP model basis vectors are undefined or invalid.
- Products are derived from Rrs. See OC_AOP: Rrs changes and known issues. Impact is improved retrieval performance, reduced scan-dependent artifacts.
- Spectral Kd has been elevated to Provisional status.

Known Issues:
- TBD

OC_BGC (Ocean Biogeochmical Properties):

Provisional Products
- Phytoplankton Chlorophyll-a (chlor_a)
- Phytoplankton Chlorophyll-a uncertainties (chlor_a_unc)
- Phytoplankton Carbon (carbon_phyto)
- Phytoplankton Carbon uncertainties (carbon_phyto_unc)
- Particulate Organic Carbon (poc)
- Particulate Inorganic Carbon (pic)

Changes from Version 3.0 to 3.1:
- Products are derived from Rrs. See OC_AOP: Rrs changes and known issues. Impact is improved retrieval performance, reduced scan-dependent artifacts.

Changes from Version 3.1 to 3.2:
- The pic product was added to the BGC suite, based on the algorithm of Mitchell et al ….

Known Issues:
- TBD

MOANA (PCCs from the Multi Ordination ANAlysis Algorithm)

Multi Ordination ANAlysis (MOANA) is a Phytoplankton Community Composition (PCC) algorithm that returns near-surface concentrations of three different phytoplankton groups: prochlorococcus, synechococcus, and picoeukaryotes. The algorithm is derived and only applied to the Atlantic ocean. It was released as a provisional product with V3.0.

Changes from Version 3.0 to 3.1:
- Products are derived from Rrs. See OC_AOP: Rrs changes and known issues.

Known Issues:
- TBD

PAR (Photosynthetically Available Radiation)

Provisional Products
- Daily Mean PAR, below-surface, scalar (par_day_scalar_below)
- Daily Mean PAR, above-surface, planar (par_day_planar_above)
- Daily Mean PAR, below-surface, planar (par_day_planar_below)
- Instantaneous PAR, above-surface, planar (ipar_planar_above)
- Instantaneous PAR, below-surface, planar (ipar_planar_below)

Changes from Version 2.0 to 3.0:
- Minor impacts from refined instrument calibration.
- Moved from Test to Provisional status.

Changes from Version 3.0 to 3.1:
- Minimal impact due to instrument and vicarious calibration updates.

Known Issues:
- TBD

CLDMASK (Cloud Mask)

Provisional Products
- Cloud Mask (cloud_flag)
- Cloud and Cloud-adjacent Mask (cloud_flag_dilated)

Changes from Version 2.0:
- Bugs have been fixed dealing with the use of the MERRA2 snow and sea ice data sets, which previously led to blockiness around coastlines.

Changes from Version 3.0 to 3.1:

- Minimal impact due to instrument ghosting correction.
- Level-3 mapped products now apply pixel area weighting, reducing data gaps.

CLD (Cloud Optical Properties and Cloud Altitude)

Provisional Products

- Cloud Top Pressure (ctp)
- Cloud Top Temperature (ctt)
- Cloud Top Height (cth)
- Cloud Optical Thickness using O_2 A-band (cth_cot)
- Cloud Effective Radius using 2.2 μm band (cer_22)
- Cloud Optical Thickness using 2.2 μm band (cot_22
- Cloud Water Path using 2.2 μm band (cwp_22)
- Cloud Effective Radius using 2.1μm band (cer_21)
- Cloud Optical Thickness using 2.1μm band (cot_21)
- Cloud Water Path using 2.1um band (cwp_21)
- Cloud Effective Radius using 1.6 μm band (cer_16)
- Cloud Optical Thickness using 1.6 μm band (cot_16)
- Cloud Water Path using 1.6 μm band (cwp_16)
- Cloud Phase using 2.1 μm band (cld_phase_21)
- Cloud Phase using 2.2 μm band (cld_phase_22)
- Cloud Phase using 1.6 μm band (cld_phase_16)

Changes from Version 2.0:

- We have expanded the cloud top product, including the COT retrieved from this algorithm (cth_cot). This algorithm (CHROMA) is independent from the CHIMAERA code used for cloud optical properties, so is a useful second estimate of COT. We have initially added a number of diagnostic retrieval outputs from the CHROMA algorithm including retrieved A-band surface albedo (cth_alb), uncertainty estimates on retrieved/derived quantities (cth_dalb, cth_dcot, cth_dcth, cth_dctp, cth_dctt), the phase retrieved by this algorithm (cth_phase), the number of iterations for convergence (cth_iter), and cost function indicating retrieval mismatch (cth_cost). Note, these diagnostic products are not provided in the L3 files.
- The 16_21 variants of cloud optical properties retrievals are no-longer produced.
- Bugs have been fixed dealing with the use of the MERRA2 snow and sea ice data sets, which previously led to blockiness around coastlines.

Changes from Version 3.0 to 3.1:

- Minimal impact due to instrument ghosting correction.
- Level-3 mapped products now apply pixel area weighting, reducing data gaps. Largest impact is to the 1-deg mapped products.

SFREFL (Surface Reflectance)

Provisional Products
- Spectral Surface Reflectance (rhos)

Changes from Version 2.0:
- The rhos product reflects the updates to OCI instrument calibration, and also includes application of the SVC gains (see OC_AOP changes). Improved performance and reduced spectral variability in the UV range is expected.
- Spectral sampling was significantly increased to include 122 spectral wavelengths between 345 nm to 2260 nm. Regions around the focal plane transition (590 – 610 nm) and in strong gas absorption regions (~690 nm and ~760 nm) have been excluded.

Changes from Version 3.0 to 3.1:
- Previous version included application of vicarious calibration gains. With the improved correction for atmospheric absorbing gases (see OC_AOP), vicarious calibration is no-longer required. Impact is reduced spectral artifacts, especially in red-NIR range.
- Cloud masking is reduced. Previous version masked data adjacent to clouds (using the "Cloud and Cloud-Adjacent" CLDMASK product, which will mask extra pixels in the vicinity of clouds and bright targets). Retrievals in cloud-adjacent pixels are now included, this increasing product coverage near clouds and coastlines.

Known Issues:
- Contribution from aerosols is not removed. Product is expected to be biased high by several percent on average.
- Bi-directional reflectance corrections are not applied, thus elevated geometric variability is to be expected.

LANDVI (Land Surface Indices)

Provisional Products
- Enhanced Vegetation Index (evi)
- Normalized Difference Vegetation Index (ndvi)
- Normalized Difference Water Index (ndwi)
- Normalized Difference Infrared Index (ndii)
- Normalized Difference Snow Index (ndsi)
- Chlorophyll-Carotenoid Index (cci)
- Carotenoid Content Index (car)
- Chlorophyll Index Red Edge (cire)
- Photochemical Reflectance Index (pri)
- Modified Anthocyanin Reflectance Index (mari)

Notes
- Multi-band indices (NDVI, EVI, NDWI, NDII, CCI, NDSI) are calculated using aggregates of OCI spectral reflectances corresponding to relevant MODIS bandwidths.

Changes from Version 2.0:
- LANDVI suite (previous called LAND) has been elevated to Provisional status.

Changes from Version 3.0 to 3.1:
- Products are derived from SFREFL. Product quality is expected to improve given reduced spectral artifacts in SFREFL.
- Coverage is increased due to decreased cloud masking in SFREFL product.

Known Issues
- The NDSI algorithm does not currently incorporate a snow impossible mask.
- Contribution from aerosols is not currently removed from surface reflectance data, which may cause residual artifacts in vegetation index calculations.

AER_UAA (Aerosol Properties from Unified Aerosol Algorithm)

This is the first release of Level-2 and Level-3 products from the Unified Aerosol Algorithm (UAA) as applied to OCI Version 3.0.1 Level-1B. The UAA algorithm generates a suite of spectral aerosol optical properties over land, ocean, and clouds, through combined heritage from the Dark Target and Deep Blue algorithms of MODIS and VIIRS and the Ultraviolet Aerosol Index (UVAI) algorithm of OMI. The algorithm operates on a 7x7 pixel average of gas-corrected reflectances from OCI, and thus the Level-2 product is at a reduced resolution relative to the Level-1B and other Level-2 products.

Provisional Products
- Aerosol Optical Depth
- Fine mode fraction of aerosol optical depth at 550 nm, over ocean

Test products
- Absorbing Aerosol Optical Depth (AAOD)
- Near-UV Aerosol Optical Depth over Cloud
- Near-UV Aerosol Index
- Near-UV Cloud Optical Depth
- Near-UV aerosol layer height
- O_2 B-band aerosol layer height
- Dark Target aerosol layer height
- Near-UV aerosol single scattering albedo (SSA)
- Dark Target aerosol single scattering albedo (SSA)
- Mean Reflectance (UV bands used)
- Mean Gas Corrected Reflectance (other bands used)

Known issues
- TBD

UVAI_UAA (UV Aerosol Index from Unified Aerosol Algorithm)

The Ultraviolet Aerosol Index (UVAI) algorithm as implemented in UAA is able to provide retrievals at the full native spatial resolution of OCI. These full resolution products are provided in a separate Level-2 file.

Provisional Products
- Near-UV Aerosol Index

Test products
- Near-UV Lambertian equivalent reflectivity (LER)
- Aerosol residue

Known issues
- TBD

OCI Level-3 Products

OCI Level-2 products are composited into global Level-3 binned and mapped products. Daily, 8-day, and monthly Level-3 mapped products are produced on an equirectanular grid at 0.1-deg and 1-deg resolution. The available list of mapped product types now include:

- RRS, AVW, FLH: apparent optical properties of ocean waters
- IOP, KD: inherent optical properties of ocean waters
- POC, CHL, CARBON: biogeochemical properties of ocean waters
- PAR: photosynthetically active radiation over water bodies
- MOANA: phytoplankton community composition of Atlantic waters, MOANA algorithm
- SFREFL: spectral quasi-surface reflectance
- LANDVI: terrestrial vegetation indices
- AER_UAA: aerosol optical properties over land, ocean, and clouds from UAA algorithm
- CLOUD: cloud optical properties from CHIMERA algorithm, cloud layer and cloud top height from Sayer et al.

SPEXone Level-1A/B/C Data (Provisional)

Changes from Version 2:

- Fixed a geolocation bug which assigned wrong latitudes and longitudes to water bodies in high elevation regions.
- Updated the algorithm for computing the Stokes Q and U and the rotation angle from the local meridian plane to the scattering plane. Whereas the degree of linear polarization was unaffected, there was ambiguity in the sign of Q and U and polarization reference planes used. In Version 3 Level-1C products, SPEXone and HARP2 use a common convention.
- Level 1C products now contain more radiance and polarization data near the poles.
- Updated bad pixel mask of the detector.

Known issues:

- A positive radiometric bias (~2.5%) in SPEXone V3 L1C data has been identified. The source of the issue is understood, and it will be corrected in a future reprocessing (V4).
- Improvement of radiometric and polarimetric performance at the edges of the wavelength grid under investigation.

SPEXone Level-2 Products

AER_RTAPOCEAN (Aerosol Properties over Ocean from RemoTAP Algorithm)
AER_RTAPLAND (Aerosol Properties over Land from RemoTAP Algorithm)

This is the first release of Level-2 and Level-3 products from the RemoTAP algorithm as applied to SPEXone Version 3 Level-1C. The RemoTAP algorithm generates a large suite of aerosol optical and microphysical properties and surface properties, including but not limited to the products listed below. The Level-2 data over ocean and land surfaces are separated into different files, but the suite of products in each is identical.

Provisional Products

- Aerosol Optical Thickness (aot)
- Single Scattering Albedo (ssa)
- Effective Radius of Fine Mode Aerosols (reff_fine)
- Effective Radius of Coarse Mode Aerosols (reff_coarse)
- Fine Mode Fraction (fmf)
- Fine Mode Fraction by Volume (fvf)
- Real Index of Refraction (mr)
- Imaginary Index of Refraction (mi)

Known issues

- Because of a positive radiometric bias (~2.5%) in SPEXone V3 L1C data, the retrieved SSA has a positive bias of 0.01-0.02.

MAPOL_OCEAN (Aerosol and Ocean Properties from FastMAPOL Algorithm)

This is the first release of Level-2 and Level-3 products from the FastMAPOL algorithm as applied to SPEXone Version 3 Level-1C. The FastMAPOL algorithm generates a large suite of aerosol and ocean properties. A subset is listed here.

Provisional Products

- Aerosol Optical Thickness (aot)
- Single Scattering Albedo (ssa)
- Effective Radius of Fine Mode Aerosols (reff_fine)
- Effective Radius of Coarse Mode Aerosols (reff_coarse)
- Fine Mode Fraction (fmf)
- Fine Mode Fraction by Volume (fvf)
- Real Index of Refraction (mr)
- Imaginary Index of Refraction (mi)
- Wind Speed (wind_speed)
- Chlorophyll a Concentration (Chla)
- Angular Remote Sensing Reflectance before BRDF correction (Rrs1)
- Angular Remote Sensing Reflectance after BRDF correction (Rrs2)

Known issues

- Small negative Rrs offset (~-0.001) is often observed at wavelengths > 600 nm.
- BRDF correction does not fully remove Rrs angular dependence (as seen in Rrs2).
- High Rrs bias at 678 nm likely due to influence of the Oxygen A-band.

SPEXone Level-3 Products

SPEXone Level-2 products are composited into global Level-3 binned and mapped products. Daily, 8-day, and monthly Level-3 mapped products are produced on an equirectanular grid at 0.1-deg and 1-deg resolution. The available list of mapped product types now include:

- AER_RTAP: aerosol optical and microphysical properties over land and ocean from RemoTAP algorithm
- AER_RTAPLAND: retrieved land surface parameters (Ross-Li)
- AER_RTAPOCEAN: retrieved ocean surface parameters (phytoplankton chlorophyll)
- MAPOL_OCEAN: aerosol and ocean properties over ocean from FastMAPOL algorithm

HARP2 Level-1A/B/C Data (Provisional)

On-orbit calibration data has been collected during solar and lunar calibration exercises, and a refined calibration is included in the version 3 release.

Changes from Version 2 to Version 3:

- For Level-1A data products, removed a x2 scaling to the AST4 (i.e., science acquisition) detector counts that was used in previous Level -1A versions, so that the detector count values are consistent across different HARP2 operations modes (i.e., between calibration and science).
- Updated radiometric coefficients, spectral center/FWHM, non-linear correction, based on a refined pre-launch calibration.
- Improved pixel defect masking to reduce vertical stripes in pushbroom images.
- Polarimetric calibration matrices (used for determining polarization from HARP2's three sensors) are expanded to full detector, whereas detector center characterization was used in previous versions. This change improves the polarization accuracy for off-nadir views.
- Improved stray light correction for off-nadir views based on extended analysis on the pre-lunch calibration.
- Applied dynamic flatfield and dark corrections based on frequent onboard solar and dark calibration, which replaced the static dark/flatfield onboard calibration characterized at beginning of the mission.
- Improved geolocation and multi-view co-registration.

Known issues

- Vertical fringes exist in the polarization (i.e., Q, U, and DoLP) pushbrooms for some view angles. These are mainly driven by uncertainty in detector flatfield (<1%).
- A geometrical-dependent bias of polarization exists in large view (zenith angle over 50 degrees from space). This is potentially caused by inaccurate stray-light correction and/or complex view-dependent polarimetric calibration at the edge of the detectors.
- Some level of false polarization due to imperfect detector alignment with current correction, which are more noticeable in nadir views.
- Error in geolocation still exists for far angles (over 50 degrees), which can exceed 1 pixel.

HARP2 Level-2 Products

MAPOL_OCEAN (Aerosol and Ocean Properties from FastMAPOL Algorithm)

This is the first release of Level-2 and Level-3 products from the FastMAPOL algorithm as applied to HARP2 Version 3 Level-1C. The FastMAPOL algorithm generates a large suite of aerosol and ocean optical properties. A subset is listed here.

Provisional Products

- Aerosol Optical Thickness (aot)
- Single Scattering Albedo (ssa)
- Effective Radius of Fine Mode Aerosols (reff_fine)
- Effective Radius of Coarse Mode Aerosols (reff_coarse)
- Fine Mode Fraction (fmf)
- Fine Mode Fraction by Volume (fvf)
- Real Index of Refraction (mr)
- Imaginary Index of Refraction (mi)
- Wind speed (wind_speed)
- Chlorophyll a concentration (Chla)
- Angular Remote Sensing Reflectance before BRDF correction (Rrs1)
- Angular Remote Sensing Reflectance after BRDF correction (Rrs2)

Known issues

- Aerosol optical depth is biased high (~0.07) as compared with AERONET-OC.
- Remote-sensing reflectance (Rrs) is biased low (-0.001) as compared with AERONET-OC.
- High uncertainty in aerosol microphysical retrievals (mr, mi, sph, alh etc).
- Fewer polarization measurements than radiance measurements are successfully fitted, as indicated by valid angle counts (Nv_ref and Nv_dolp) and angular data mask (mask_ref and mask_dolp).

CLOUD_GPC (Cloud Properties from GISS Polarimetric Cloud Algorithm)

This is the first release of Level-2 and Level-3 products from the GISS Polarimetric Cloud (GPC) algorithm, applied to HARP2 Version 3 Level-1C. The GPC algorithm produces a suite of cloud properties using three polarimetric cloud retrievals techniques, along with additional cloud properties derived by combining them with selected OCI L2 CLD retrievals. Selected additional variables from OCI L2 CLD are also included. A subset is listed here.

Provisional Products

- cloud_bow_droplet_effective_radius
- cloud_bow_droplet_effective_variance
- cloud_bow_rms
- cloud_bow_fit_correlation
- cloud_bow_quality_retrieval_fail
- cloud_liquid_index
- cloud_rft_mode_fraction_0
- cloud_rft_mode_fraction_1

- cloud_rft_quality_retrieval_fail

Known issues

- Retrieval artifacts associated with L1C polarization—particularly those related to rotation plane and angle—are present but are expected to improve as the L1C polarization calibration effort progresses.
- Early versions of RFT retrievals are intended primarily for exploratory purposes to support algorithm refinement. Larger biases and other issues are expected in RFT retrievals compared to parametric retrievals.

HARP2 Level-3 Products

HARP2 Level-2 products are composited into global Level-3 binned and mapped products. Daily, 8-day, and monthly Level-3 mapped products are produced on an equirectanular grid at 0.1-deg and 1-deg resolution. The available list of mapped product types now include:

- MAPOL_OCEAN: aerosol and ocean properties over ocean from FastMAPOL algorithm
- CLOUD_GPC: cloud properties from GPC algorithm

Appendices

Data Levels and Formats:

As in previous versions, all data products are distributed in self-describing netCDF4 format and are available in the following data processing levels.

- Level-1A, raw instrument data and spacecraft telemetry, reformatted to netCDF4
- Level-1B, calibrated & geolocated instrument data
- Level-1C, calibrated, geolocated, and co-registered to a common grid
- Level-2, derived geophysical science data products
- Level-3, temporally and spatially composited (binned and mapped) global products
- Level-4, geophysical products derived from combined Level-3 inputs and/or models

Level-1C and Level-2 data files are divided into 5-minute granules that start at the southern terminator crossing of the ascending daylight orbit and end at the northern terminator crossing. For OCI, and HARP2 the Level-1A and Level-1B data are also in 5-minute granules, while SPEXone is organized into continuous daylight orbit periods (~50 minutes).

Level-3 products are generally global daily, 8-day, or monthly composites that are distributed in multiple spatial resolutions, including 4.6km, 0.1-deg, and 1.0-deg maps (Level-3m). A single L3m file may contain one 2D mapped product, or one 3D cube (e.g., where the 3rd dimension is the spectral dimension), or multiple 2D and/or 3D mapped products. The mapped products are derived by reprojection of binned data (Level-3b), where the typical bin distribution is a quasi-equal-area 4.6km or 9.2km integerized sinusoidal grid.

The products available are categorized into maturity levels as:

- Provisional: results have been reviewed and are in family with heritage data products or other basis of expectation, but which have not yet been validated and may still contain significant errors.
- Test: results have not yet been reviewed by algorithm developers and or may be known to have substantial errors in implementation that are under investigation.
- Diagnostic: products that are produced to support analysis of algorithm behavior, but that are not intended for science.

PACE Science Data Reprocessing Version 2

The notes that follow provide an overview of the changes introduced between Version 1 and Version 2, for the Level-1 products of each instrument as well as the derived science products currently available. For a comprehensive list of the science data products planned for PACE and the current status of those products and algorithms see the PACE Data Products Table.

OCI Level-1A/B/C Data (Provisional)

Changes from Version 1:

- The OCI absolute calibration coefficients were revised by combining on-orbit solar diffuser measurements and prelaunch GLAMR measurements. The solar diffuser based calibration coefficients below 900nm are adjusted to agree with the longer range spectral trends of the GLAMR coefficients, eliminating noise that was apparent in the GLAMR coefficients regarding mirror side ratios and adjacent spectral channels. Calibration coefficients of the SWIR channels are purely based on solar diffuser measurements, because a hysteresis correction has not yet been applied to the prelaunch data. The SWIR band calibration will be updated in a future reprocessing.
- Geolocation accuracy was significantly improved and is now within 1 pixel at all scan angles.
- The bug in SWIR band L1B processing that caused invalid values in the first scan line of each file was resolved.

Known Issues and Data Characteristics:

- The optical design of the OCI SWIR detector assembly (SDA) causes the bands to view different locations along-scan at a given time, and the data are packetized by time. The bands are pixel-shifted into alignment with the hyperspectral bands. This results in fill pixels at the start or end of the scan, depending on the required pixel shift. The worst case is the 2260 nm band that has 13 fill pixels at the start of the scan.
- Data below 340nm has not been characterized prelaunch as completely and accurately as the data above 340nm. The data below 340nm is only released to facilitate assessment and potential refinement of radiometric accuracy and should not be considered as science quality.
- Data in the transition region between the red and blue focal planes, between 590 and 610nm, shows significant discontinuity. The discrepancy varies with mirror side and possibly with scan angle. Measurements in this range have much higher uncertainty and should not be used for science algorithms.
- Some SWIR bands show significant signs of apparent band-to-band registration issues. SWIR data (especially bands 1038nm, 1250nm Standard Gain, and 1615nm Standard Gain) with large radiance gradients to neighboring pixels in scan direction.

- The temporal gain trend of the calibration in this update is derived from measurements of the daily solar diffuser (SD) measurements, assuming that the SD reflectance is stable. In a future update, the monthly solar diffuser measurements will be used to reduce the impact of changes in solar diffuser reflectance on the trend in measured top-of-atmosphere radiances. The impact will likely be small above 450nm (<0.2%), but larger at shorter wavelengths.
- Occasional noise spikes are seen in OCI dark data, especially in the area of the Southern Atlantic Anomaly. These spikes corrupt the background subtraction for a complete scan line, leading to striping in the L1B data. The algorithm to calculate the background subtraction in the L1B code will be improved to remove these noise spikes in the next reprocessing. It is likely that similar noise spikes are present in individual pixels of the earth view data as well. Handling earth view noise spikes will be a longer term effort.
- Further improvements in geolocation accuracy are on-going. It has been determined that the PACE spacecraft on-board ephemerous data currently used for geolocation of OCI produces uncertainties of order 150 meters. This will be resolved in refined processing through use of definitive ephemeris data derived in ground-based post processing of the GPS data.

HARP2 Level-1A/B/C Data (Provisional)

On-orbit calibration data has been collected during solar and lunar calibration exercises, and a refined calibration is included in the version 2 release.

Changes from Version 1:
- Improvements to instrument calibration based on data collected during on-orbit solar and lunar calibration exercises. This includes:
    - Correction for elevated brightness observed in V1
    - Refined, FOV-dependent radiometric & polarimetric characterization
    - Updated dark offsets
    - V2 results are now within +/-3% in comparison with OCI (subject to verification, one-sigma)
- Geolocation accuracy now within one Level-1B pixel for all angles through:
    - Improved optical model (spectral-dependent magnification & distortion, realistic MTDI sampling)
    - Improved HARP2 boresight offsets
- Improved detector alignment for reducing false polarization

Known issues
- Polarimetric performance is subject to comprehensive evaluation, particularly in the accuracy of DoLP and reference plane orientation.

- Blue band exhibits both positive and negative bias relative to other bands when compared with SPEXOne over multiple orbits spanning several days. This bias is dependent on the viewing angle and latitude. Efforts are currently underway to investigate the origins of this bias and to develop appropriate corrections.
- The red scale factor trends higher than the non-red factor by about 25%. This will result in a larger subtraction of the red data as compared to the non-red data. This will affect the radiometric data and we need to test the new correction.
- Geolocation performance is subject to more comprehensive evaluation.
- Alignment related false polarization needs further evaluation and improvement

SPEXone Level-1A/B/C Data (Provisional)

Changes from Version 1:
- Geolocation accuracy has been improved.
- Additional bad detector pixels have been identified and masked.
- Unphysical oscillations in the degree of polarization (DoLP) and radiance have been reduced by applying a small shift to the detector image.
- Radiometric response accuracy has been improved.

Known issues:
- Reduced DoLP accuracy at the shortest wavelengths.

OCI Level-2 Products

An expanded set of OCI Level-2 science data products is being released at this time. They are organized into product suites, with each suite in one file per granule. In some cases, the Level-2 products suites contain a mix of Provisional, Test, and Diagnostic products.

OC_AOP, Ocean Color Apparent Optical Properties:

Provisional Products
- Remote Sensing Reflectance (Rrs)
- Rrs Uncertainties (Rrs_unc)

Test Products
- Apparent Visible Wavelength (avw)

Diagnostic Products
- Aerosol Optical Thickness (aot)
- Aerosol Angstrom Exponent (angstrom)

Changes from Version 1.0:

- The updated absolute calibration of OCI increased the magnitude of Rrs retrievals in all wavelengths above 400nm, and significantly reduced suspect band-to-band spectral variability. Mirror-side striping artifacts are also substantially reduced.
- An updated atmospheric gas transmittance correction that now includes effects of O2-O2 collision-induced absorption resulted in reduced residual gas transmittance artifacts in the Rrs retrievals (e.g., near 360, 380, 477, 577, and 630nm).
- Data are now flagged as reduced quality for view zenith angles greater than 60-deg. These flagged data are masked in Level-3 products. In V1 the data was flagged at 75-deg, and thus extended to the edge of the OCI swath.
- Data within 1 pixel along track and within 2 pixels across track from a bright source such as a cloud are flagged as reduced quality, based on pre-launch characterization of bright source recovery (e.g., straylight). These straylight flagged pixels are masked in Level-3 products. No straylight flagging was done in V1.

Known Issues:

- No vicarious calibration has yet been applied. It is expected that a vicarious calibration will be applied in the next reprocessing, to reduce bias in the Rrs retrievals relative to ground truth.
- Performance of Rrs retrieval in the UV (below 400nm) has not yet been meaningfully reviewed and is likely to contain significant biases and erroneous variability.
- Corrections for absorbing gases have been applied, but refinement is on-going. Rrs variability, especially in the red, is likely to contain residual artifacts from water vapor and oxygen absorption near 680nm, 720nm, 760nm, and 820nm.
- As noted above, there is a discontinuity in the observed radiances at the transition between the blue and red focal planes. This results in an artifact in Rrs in the 590-610nm region. Science algorithms should avoid use of data in this region.
- The current processing extends to higher view zenith angles than the heritage sensors. The atmospheric correction becomes increasingly difficult at these extreme geometries, and erroneously elevated reflectance has been observed in red wavelengths near scan edge. These data are flagged at Level-2 and masked at Level-3.
- Chlorophyll Fluorescence Line Height will be included in a future release.

OC_IOP (Ocean Inherent Optical Properties):

Provisional Products

- Total absorption coefficient (a)
- Total backscatter coefficient (bb)
- Phytoplankton absorption coefficient (aph)
- Phytoplankton absorption coefficient standard uncertainty (aph_unc)
- Non-algal particle plus chromophoric dissolved organic matter absorption coefficient (adg)

- Non-algal particle plus chromophoric dissolved organic matter absorption coefficient standard uncertainty (adg_unc)
- Particle backscattering coefficient (bbp)
- Particle backscattering coefficient standard uncertainty (bbp_unc)

Test Products
- Spectral diffuse attenuation coefficient (Kd)

Diagnostic Products
- Mean residual of model fit (rrsdiff)

Changes from Version 1.0:

Known Issues:
- Products are derived from Rrs. See OC_AOP: Rrs known issues.
- Some algorithm failure and artifacts noted in highly productive and near-shore waters. Future refinement will improve these missing data.

OC_BGC (Ocean Biogeochmical Properties):

Provisional Products
- Phytoplankton Chlorophyll-a (chlor_a)
- Phytoplankton Chlorophyll-a uncertainties (chlor_a_unc)

Test Products
- Phytoplankton Carbon (carbon_phyto)
- Phytoplankton Carbon uncertainties (carbon_phyto_unc)
- Particulate Organic Carbon (poc)

Changes from Version 1.0:

Known Issues:
- Products are derived from Rrs. See OC_AOP: Rrs known issues.
- Circular artifacts observed near subsolar point, where OCI is tilting through nadir and glint is extreme. Future refinement will improve or mask these artifacts.
- Particulate Inorganic Carbon (pic) and poc_unc will be included in a future release.

PAR (Photosynthetically Available Radiation)

Test Products
- Daily Mean PAR, Below-surface, Scalar (par_day_scalar_below)

- Daily Mean PAR, Above-surface, Planar (par_day_planar_above)
- Daily Mean PAR, Below-surface, Planar (par_day_planar_below)
- Instantaneous PAR, Below-surface, Planar (ipar_planar_above)
- Instantaneous PAR, Below-surface, Planar (ipar_planar_below)

Changes from Version 1.0:

Known Issues:

CLDMASK (Cloud Mask)

Test Products
- Cloud Mask (cloud_flag)
- Cloud and Cloud-adjacent Mask (cloud_flag_dilated)

Changes from Version 1.0:
- This is the first public release for these products.

CLD (Cloud Optical Properties and Cloud Altitude)

Test Products
- Cloud Top Pressure (ctp)
- Cloud Top Temperature (ctt)
- Cloud Top Height (cth)
- Cloud Effective Radius using 2.2 μm band (cer_22)
- Cloud Optical Thickness using 2.2 μm band (cot_22
- Cloud Water Path using 2.2 μm band (cwp_22)
- Cloud Effective Radius using 2.1μm band (cer_21)
- Cloud Optical Thickness using 2.1μm band (cot_21
- Cloud Water Path using 2.1um band (cwp_21)
- Cloud Effective Radius using 1.6 μm band (cer_16)
- Cloud Optical Thickness using 1.6 μm band (cot_16)
- Cloud Water Path using 1.6 μm band (cwp_16)
- Cloud Effective Radius using 1.6 μm and 2.1 μm bands (cer_16_21)
- Cloud Optical Thickness using 1.6 μm and 2.1 μm bands (cot_16_21)
- Cloud Water Path using 1.6 μm and 2.1 μm bands (cwp_16_21)
- Cloud Phase using 2.1 μm band (cld_phase_21)
- Cloud Phase using 2.2 μm band (cld_phase_22)
- Cloud Phase using 1.6 μm band (cld_phase_16)
- Cloud Phase using 1.6 μm and 2.1 μm bands (cld_phase_16_21)

Changes from Version 1.0:
- This is the first public release for these products.

SFREFL (Surface Reflectance)

Test Products
- Spectral Surface Reflectance (rhos)

Changes from Version 1.0:
- This is the first public release for these products.

Notes:
- Surface reflectances are currently produced using the L2gen algorithm.

Known Issues:
- Data is limited to 50 spectral wavelengths between 339nm to 2260nm.
- Contribution from aerosols is not removed.
- Residual artifacts in the spectral vicinity of strong atmospheric gas absorption (e.g., water vapor and oxygen) is expected.
- Data is cloud masked using the “Cloud and Cloud-Adjacent" CLDMASK product, which will mask extra pixels in the vicinity of clouds and bright targets.

LAND (Land Surface Indices)

Test Products
- Enhanced Vegetation Index (evi)
- Normalized Difference Vegetation Index (ndvi)
- Normalized Difference Water Index (ndwi)
- Normalized Difference Infrared Index (ndii)
- Normalized Difference Snow Index (ndsi)
- Chlorophyll-Carotenoid Index (cci)
- Carotenoid Content Index (car)
- Chlorophyll Index Red Edge (cire)
- Photochemical Reflectance Index (pri)
- Modified Anthocyanin Reflectance Index (mari)

Notes
- Multi-band indices (NDVI, EVI, NDWI, NDII, CCI, NDSI) are calculated using aggregates of OCI spectral reflectances corresponding to relevant MODIS bandwidths.

Changes from Version 1.0:

- This is the first public release for these products.

Known Issues

- The NDSI algorithm does not currently incorporate a snow impossible mask.
- Contribution from aerosols is not currently removed from surface reflectance data, which may cause residual artifacts in vegetation index calculations.
- Data is cloud masked using the “Cloud and Cloud-Adjacent" product, which will mask extra pixels in the vicinity of clouds and bright targets.

For Future Release – Not To Be Included In Public Release Notes

AER_DT (Aerosol Properties using Dark Target Algorithm)

Test Products

- Fine Mode Fraction at 550nm (fmf_550_db)
- Aerosol Angstrom Exponent (angstrom_db)
- Aerosol Type (aerosol_typ_db)
- Aerosol Optical Thickness at 380nm (aot_380_db)
- Aerosol Optical Thickness at 410nm (aot_410_db)
- Aerosol Optical Thickness at 490nm (aot_490_db)
- Aerosol Optical Thickness at 550nm (aot_550_db)
- Aerosol Optical Thickness at 670nm (aot_670_db)
- Aerosol Optical Thickness at 865nm (aot_865_db)
- Aerosol Optical Thickness at 1240nm (aot_1240_db)
- Aerosol Optical Thickness at 1610nm (aot_1610_db)
- Aerosol Optical Thickness at 2250nm (aot_2250_db)

Known Issues:

- Heritage algorithm implemented by PACE for testing purposes only (not reviewed by original algorithm developers).

AER_DB (Aerosol Properties using Deep Blue Algorithm)

Test Products

- Fine Mode Fraction at 550nm (fmf_550_db)
- Aerosol Angstrom Exponent (angstrom_db)
- Aerosol Type (aerosol_typ_db)
- Aerosol Optical Thickness at 380nm (aot_380_db)
- Aerosol Optical Thickness at 410nm (aot_410_db)

- Aerosol Optical Thickness at 490nm (aot_490_db)
- Aerosol Optical Thickness at 550nm (aot_550_db)
- Aerosol Optical Thickness at 670nm (aot_670_db)
- Aerosol Optical Thickness at 865nm (aot_865_db)
- Aerosol Optical Thickness at 1240nm (aot_1240_db)
- Aerosol Optical Thickness at 1610nm (aot_1610_db)
- Aerosol Optical Thickness at 2250nm (aot_2250_db)

Known Issues:

- Heritage algorithm implemented by PACE for testing purposes only (not reviewed by original algorithm developers).