PACE
Ocean Products

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PACE Ocean

why do we care

• Ocean (and life in it) control climate
• Ocean (and life in it) is a critical part of the world's economy
• Phytoplankton:
  • Base of marine food web
  • Produces oxygen that we breathe
  • Draws down carbon dioxide (and assists with anthropogenic CO₂ drawdown)

*What makes PACE super special is that it will be observing ocean & atmosphere together – two Earth systems that are interlinked in so many ways.*
SPECTRAL REMOTE SENSING REFLECTANCES
SPECTRAL DIFFUSE ATTENUATION COEFFICIENTS
SPECTRAL PHYTOPLANKTON ABSORPTION COEFFICIENTS
SPECTRAL NON-ALGAL PARTICLE PLUS DISSOLVED ORGANIC MATTER ABSORPTION COEFFICIENTS
SPECTRAL CHROMOPHORIC DISSOLVED ORGANIC MATTER ABSORPTION COEFFICIENTS
SPECTRAL SLOPE COEFFICIENTS OF CHROMOPHORIC DISSOLVED ORGANIC MATTER ABSORPTION
SPECTRAL PARTICLE BACKSCATTERING COEFFICIENTS
FLUORESCENCE LINE HEIGHT
DAILY PHOTOSYNTHETICALLY AVAILABLE RADIATION (PAR)
INSTANTANEOUS PHOTOSYNTHETICALLY AVAILABLE RADIATION (iPAR)
CONCENTRATION OF CHLOROPHYLL-A
PHYTOPLANKTON PIGMENT CONCENTRATIONS
NET PRIMARY PRODUCTION (NPP)
PHYTOPLANKTON COMMUNITY COMPOSITION
CONCENTRATION OF PARTICULATE ORGANIC CARBON
CONCENTRATION OF PARTICULATE INORGANIC CARBON
CONCENTRATION OF PHYTOPLANKTON CARBON
CONCENTRATION OF DISSOLVED ORGANIC CARBON
SUSPENDED PARTICULATE MATTER
OTHER COOL THINGS YOU NEED TO FIGURE OUT

Required PACE ocean (OCI) products

Products we want for PACE (advanced)
PACE Ocean Color Atmospheric correction from OCI

Amir Ibrahim
Ocean color is the measurement of the spectral distribution of radiance (or reflectance) upwelling from the ocean in the visible regime. IOCCG

What causes variation in the color of the ocean?

The color of the ocean is a function of light that is absorbed or scattered as a result of constituents in the water.

- Phytoplankton and pigments
- Dissolved organic matter
- Detritus (fecal pellets, dead cells)
- Inorganic particles (sediment)
- Water absorption

Water-leaving Reflectance
What do we observe from a spaceborne sensor?

True color images from MODIS-Aqua - September 17, 2021
What do we observe from a spaceborne sensor?
Ocean Color is a passive remote sensing technique.

Light reaching the satellite = Light in the atmosphere + Light reflected off the ocean + Water-leaving component of light

"Atmospheric correction"

OCI MODIS

Light

Solar radiation

Atmospheric component

Surface reflection

Water-leaving component

Oceanic contribution

One scientist's noise is another's signal
Remote sensing reflectance ($R_{rs}$; sr$^{-1}$)

\[
R_{rs} = \frac{\text{upwelling radiance}}{\text{downwelling irradiance}} = \frac{L_w}{E_d}
\]

$L_w$ (Wm$^2$μm sr$^{-1}$)  \hspace{1cm}  $E_d$ (Wm$^2$μm)

$\rho_w = \pi R_{rs}$ (unitless)

Downwelling irradiance (at the surface)

Upwelling radiance (just above)
Requirements for $R_{rs}$ ($\rho_w = \pi R_{rs}$)

<table>
<thead>
<tr>
<th>Data Product</th>
<th>Baseline Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water-leaving reflectances centered on (±2.5 nm) 350, 360, and 385 nm (15 nm bandwidth)</td>
<td>0.0057 or 20%</td>
</tr>
<tr>
<td>Water-leaving reflectances centered on (±2.5 nm) 412, 425, 443, 460, 475, 490, 510, 532, 555, and 583 (15 nm bandwidth)</td>
<td>0.0020 or 5%</td>
</tr>
<tr>
<td>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)</td>
<td>0.0007 or 10%</td>
</tr>
</tbody>
</table>

Atmospheric Correction using OCI alone

*Better characterization of aerosols using MAP

Additional required products to be generated
- Chlorophyll concentration
- Spectral diffuse attenuation coefficients
- Spectral absorption coefficients (phytoplankton, CDOM+NAP)
- Spectral backscattering coefficients
- Fluorescence line height

These are required for mission success & drive OCI design

Each uncertainty requirement is defined as the maximum absolute and relative values for Level-2 satellite data processing (geophysical values in the original satellite coordination system). These requirements are specified for ≥ 50% of the observable deep ocean (≥ 1000 m).
Atmospheric Correction

- Molecular scattering removal
- Aerosol scattering + absorption correction (black pixel assumption)
- Absorbing gases compensation
- Surface glint correction

\[ L_t(\lambda) = \left( L_r(\lambda) + L_a(\lambda) + L_{ra}(\lambda) + t(\lambda) L_f(\lambda) + T(\lambda) L_g(\lambda) + t(\lambda) L_w(\lambda) \right) \times T_g(\lambda) \]
Formulation

\[
L_t(\lambda) = \left( L_r(\lambda) + L_\alpha(\lambda) + L_{\alpha\alpha}(\lambda) \right) + t(\lambda)L_f(\lambda) + T(\lambda)L_g(\lambda) + t(\lambda)L_w(\lambda) \right) \times T_g(\lambda)
\]
NASA’s operational AC algorithm

\[ L_t(\lambda) = \left(L_r(\lambda) + L_a(\lambda) + L_{ra}(\lambda) + t(\lambda)L_f(\lambda) + T(\lambda)L_g(\lambda) + t(\lambda)L_w(\lambda)\right) \times T_g(\lambda) \]

\[ \rho \neq \rho' \neq \rho'' \]

From L0

L1B calibrated top of atmosphere spectral reflectance (i.e. HICO, OCI)

Sensor specific tables for Rayleigh and aerosols

Ancillary data Pressure, RH, wind speed, ozone, NO2

f_gain

\[ \rho_t \]

\[ \rho_r, \rho_a, \rho_{ra} \]

8 gases → (H2O, O3, O2, NO2, N2O, CH4, CO2, CO)

\[ O_3, RH, WS, P, NO_2 \]

\[ T_g \]

\[ \nu \rho_w \]

\[ \nu \rho_w' \]

\[ \nu \rho_w'' \]

L2GEN

L2gen AC processing module

Implementation

\[ \nu \]

in – situ \( \rho_w \)

\[ \nu \]

To L3

Level 2 products, [Chl], Rrs, Es, a, bb, water vapor, etc.

Vicariously calibrated Level 2 products, [Chl], Rrs, Es, a, bb, water vapor, etc.

Vicarious calibration

in-situ reflectance at just above sea surface (i.e. MOBY)

Validation
Rayleigh scattering $L_r(\lambda)$

- Using a vector radiative transfer code, Lookup Tables are generated and stored to perform the Rayleigh correction.
- Permutated set of:
  - Solar zenith.
  - Sensor zenith.
  - Relative azimuth.
  - Windspeed.
- Surface pressure.

$$L_t(\lambda) = \left( L_r(\lambda) + L_\alpha(\lambda) + L_{r\alpha}(\lambda) + t(\lambda)L_f(\lambda) + T(\lambda)L_g(\lambda) + t(\lambda)L_w(\lambda) \right) \times T_g(\lambda)$$

\[\theta_0 = 60^\circ, \theta = 20^\circ, \Delta = 90^\circ\]
Gas absorption correction $T_g(\lambda)$

Hawaii H2013050000822

Gas absorption cross sections for all gas species are calculated using the LBL HITRAN database. A table with the gas transmittances is stored and used to compensate for the gas absorption. Ancillary data of the gas concentrations are used, except for water vapor.
Direct sun glint $T(\lambda)L_g(\lambda)$
OCI tilt to avoid glint and increase coverage

OCI is tilted 20° to avoid glint

SeaWiFS PAR - June 21, 2007 (with tilt)

MODIS-Aqua PAR - June 21, 2007 (without tilt)

PAR = Photosynthetically Available Radiation
White caps $t(\lambda)L_f(\lambda)$

\[
F_{wc} = 5.0 \times 10^{-5} (U_{10} - 4.47)^3 \quad \text{for developed seas}
\]
\[
F_{wc} = 8.75 \times 10^{-5} (U_{10} - 6.33)^3 \quad \text{for undeveloped seas}
\]

\[
[rho_{wc}]_N(\lambda) = a_{wc}(\lambda) \times 0.22 \times F_{wc}
\]
\[
= a_{wc}(\lambda) \times 1.925 \times 10^{-5} (U_{10} - 6.33)^3
\]

\[
L_t(\lambda) = (L_r(\lambda) + L_a(\lambda) + L_{ra}(\lambda) + t(\lambda)L_f(\lambda) + T(\lambda)L_g(\lambda) + t(\lambda)L_w(\lambda)) \times T_g(\lambda)
\]
Aerosols challenge

- Complex morphology.
- Chemical composition.
- Size distribution.

Kokhanovsky et al., 2015
This simulation used GEOS-5 and the Goddard Chemistry Aerosol Radiation and Transport (GOCART) Model.
Aerosol microphysical model

Ahmad et al., 2010

\[
L_t(\lambda) = (L_r(\lambda) + L_a(\lambda) + L_{ra}(\lambda) + t(\lambda)L_f(\lambda) + T(\lambda)L_g(\lambda) + t(\lambda)L_w(\lambda)) \times T_g(\lambda)
\]
Aerosol LUTs $L_a(\lambda) + L_{ra}(\lambda)$

- To perform the AC, we need to generate aerosol LUTs.
- Perform multidimensional linear interpolation for each pixel of the granule.
- Dimensions of aerosol reflectance ($\rho_a$) LUT:
  - relative humidity (rh): 8
  - fine-mode fractions (fmf): 10
  - optical depth ($\tau$): 9
  - wavelengths ($\lambda$): 239
  - solar zenith ($\theta_0$): 33
  - relative azimuth ($\phi$): 19
  - sensor zenith ($\theta$): 35

*Hyperspectral $L_t(\lambda) = (L_r(\lambda) + L_a(\lambda) + L_{ra}(\lambda) + t(\lambda)L_f(\lambda) + T(\lambda)L_g(\lambda) + t(\lambda)L_w(\lambda)) \times T_g(\lambda)$

$rh = 75, \tau(870) = 0.1, \theta_0 = 25, \phi = 135, \theta = 23.47$

\[ \rho_a \]

\[ \text{Wavelength (nm)} \]

~3.8 billion data point!
Black pixel assumption for aerosol correction

\[
R_{RS} \quad (\text{Sr}^{-1})
\]

Wavelength (nm)
Heritage and recent advancements in AC algorithms:

- **Gordon and Wang, 1994**
  - [Image showing graphs and data points]

- **MSEPS**
  - Ahmad et al., 2010
  - [Image showing wavelength spectrum and data points]

- **MBAC**
  - Ibrahim et al., 2019
  - [Image showing absorption coefficient spectrum and data points]

**NASA’s operational AC algorithm with focus on the aerosols correction**

- [Graph showing aerosols correction]
Multi-band Atmospheric Correction (MBAC)

TOA radiance $L_t$

Rayleigh, gas, and glint correction $L_{rgc}$

Estimate the optical depth at the longest high radiometric quality band $\tau_{a}(\lambda = 860\text{nm})$

Estimate the aerosol spectral reflectance for a set of models

Average best models, calculate transmittances $R_{rs}, \tau_a, \text{Ångström}$

$\nabla \chi^2$ minimization

$Ibrahim et al., 2019$

$$\chi^2(RH, f) = \frac{1}{DOF} \sum_{\lambda=860}^{850} \frac{[\rho_{obs}(\lambda) - \rho_{a}(\lambda, RH, f)]^2}{\sigma^2(\lambda)} \times SW(\lambda)$$
In turbid waters, NIR reflectance can be non-negligible. Separating the ocean signal from the atmosphere is difficult. Iterative NIR correction (Bailey et al., 2010) reduces the errors by modeling the reflectance of the ocean. Utilizing bands in the SWIR for AC significantly reduce the impact of turbid water due to the increased water absorption.

<table>
<thead>
<tr>
<th>Sensor/ Wavelength (nm)</th>
<th>MODIS</th>
<th>VIIRS</th>
<th>PACE-OCI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensor/ Wavelength (nm)</td>
<td></td>
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</tr>
<tr>
<td>MODIS</td>
<td>748</td>
<td>746</td>
<td>750</td>
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<tr>
<td></td>
<td>859</td>
<td>868</td>
<td>860</td>
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<td>2260</td>
</tr>
</tbody>
</table>

The adaptive spectral weight for each band depends on the number of iterations in the NIR algorithm. More iterations mean difficulty on converging the bio-optical model. The method allows for open ocean and coastal water processing without the need to switch between tunable algorithms (NIR AC → SWIR AC).
Application and benefits of OCI SWIR channels

- Better Atmospheric Correction in coastal waters
- Better sensitivity to turbidity and less prone to saturation than NIR.

Knaeps et al. 2015 RSE
MBAC retrievals are similar to the operational algorithm, except in turbid coastal regions.

That is due to the difference in the retrieved aerosols models.

Turbid waters over-estimate the aerosol reflectance (i.e., angstrom).
Bidirectional reflectance distribution (BRDF) correction

- The definition of $R_{rs}$ is for Sun and Zenith and sensor at Nadir.
- Pixel to pixel geometry changes thus to standardize the data, we need to apply the BRDF correction.

$$[\rho_w]_N^{ex} \equiv \frac{\pi}{F_0}[L_w]_N^{ex}$$

$$= \left\{ \frac{\pi}{F_0 \cos \theta_s t(\theta_s)} \frac{\mathcal{R}_o(W)}{\mathfrak{R}(\theta'_v, W)} \frac{f_0(\text{ATM}, W, \text{IOP})}{Q_0(\text{ATM}, W, \text{IOP})} \left[ \frac{f(\theta_s, \text{ATM}, W, \text{IOP})}{Q(\theta_s, \theta'_v, \phi, \text{ATM}, W, \text{IOP})} \right]^{-1} \right\} \times L_w(\theta_s, \theta_v, \phi).$$
Demonstration of Hyperspectral Rrs(λ) Retrieval from HICO, including correction for atmospheric water vapor

Example over Lake Erie. In-situ measurements provided by Tim Moore (UNH), obtained from SeaBASS
Putting it all together
Testing HS AC on simulated OCI data

Example retrieval of $R_{rs}$ from PyTOAST simulations
HS AC from airborne data - AVIRIS

Aeronet-OC WaveCIS – Gulf of Mexico
Challenges and opportunities with PACE

**Challenges**

- Strongly absorbing and non-spherical aerosols. Aerosol vertical profile.
- UV atmospheric signal is too large.
- UV IOPs and BRDF correction needs further improvements.
- Improve bio-optical modeling in the NIR-SWIR.
- Improved gas correction (coupling scattering-absorption)
- Adjacency effects.

**Opportunities**

- Great UV measurement capabilities (retrieve $O_3$, $NO_2$, absorbing aerosols, turbid water AC).
- Great SWIR performance.
- HS measurements can better constrain the AC problem.
- Synergy between OCI and MAP is unique.