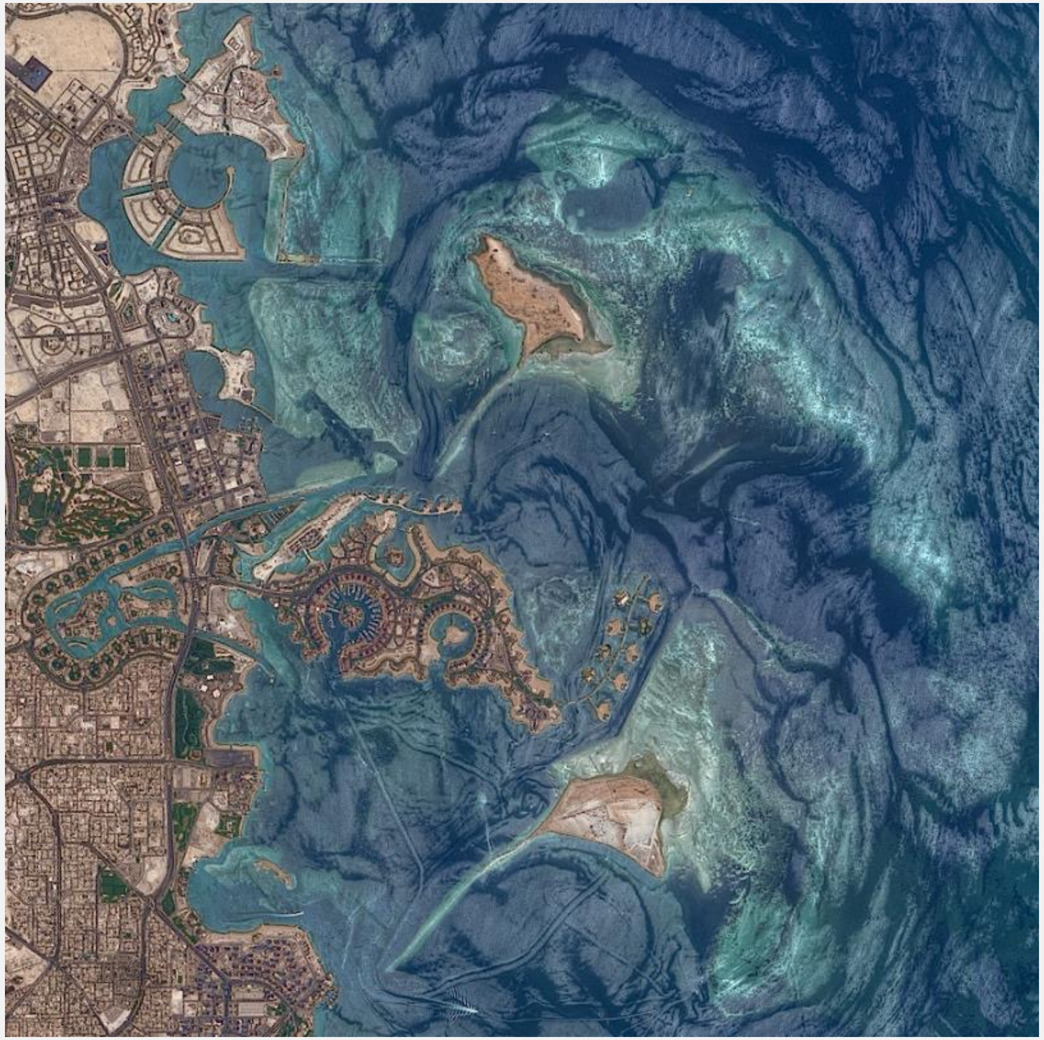
PACE Ocean Products

Amir Ibrahim, Jessie Turner, Lachlan McKinna, Ivona Cetinić
(and rest of the PACE team)

PA**C**E 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 CO_2 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.



Steampunk Qatar coastline, Landsat 9 July 24th 2022 by Norman Kuring

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

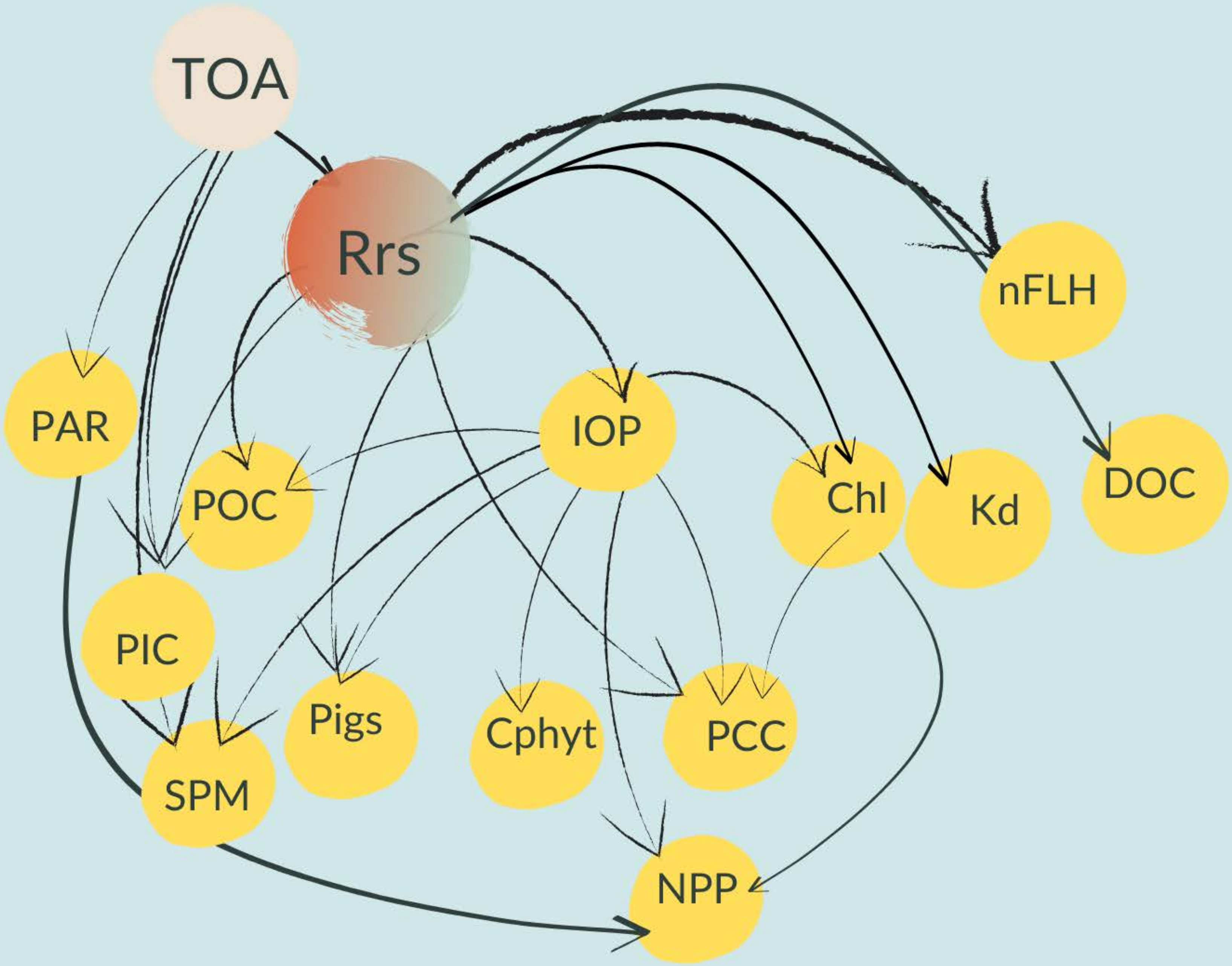
CONCENTRATION OF DISSOLVED ORGANIC CARBON

SUSPENDED PARTICULATE MATTER

OTHER COOL THINGS YOU NEED TO FIGURE OUT

Required PACE ocean (OCI) products

Products we want for PACE (advanced)


TOA
Rrs
nFLH
PAR
IOP
POC
Chl
Kd
DOC
PIC
Pigs
Cphyt
PCC
SPM
NPP

PACE Ocean Color Atmospheric correction from OCI

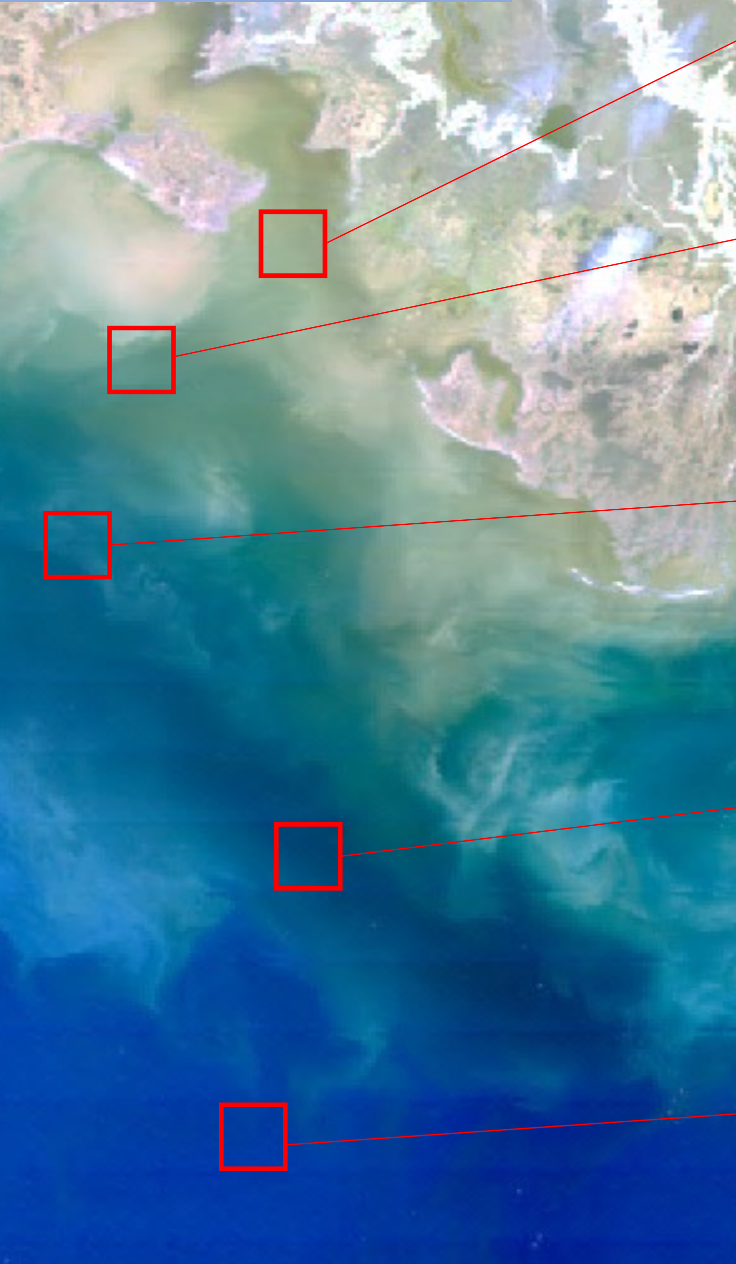
Amir Ibrahim

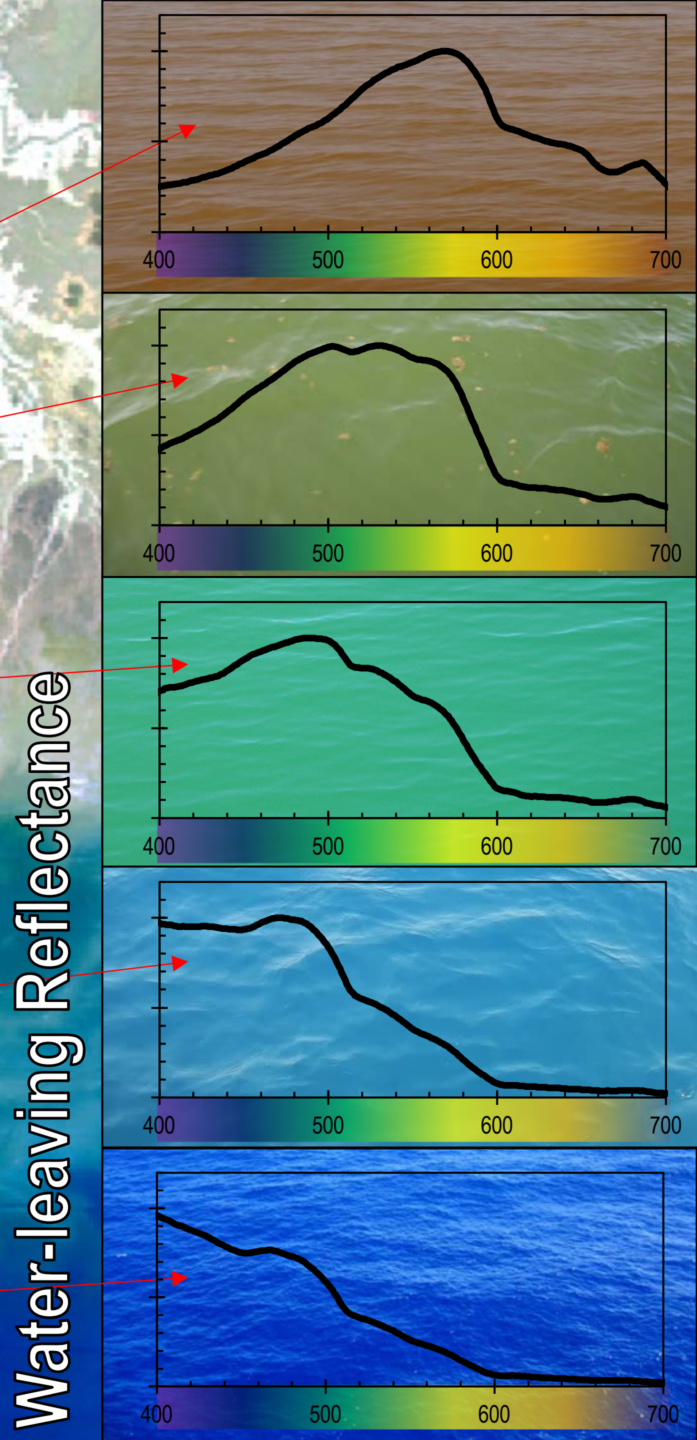
Ocean color is the measurement of the spectral distribution of radiance (or reflectance) upwelling from the ocean in the visible regime. IOCCG

What causes variation in the color of the ocean?

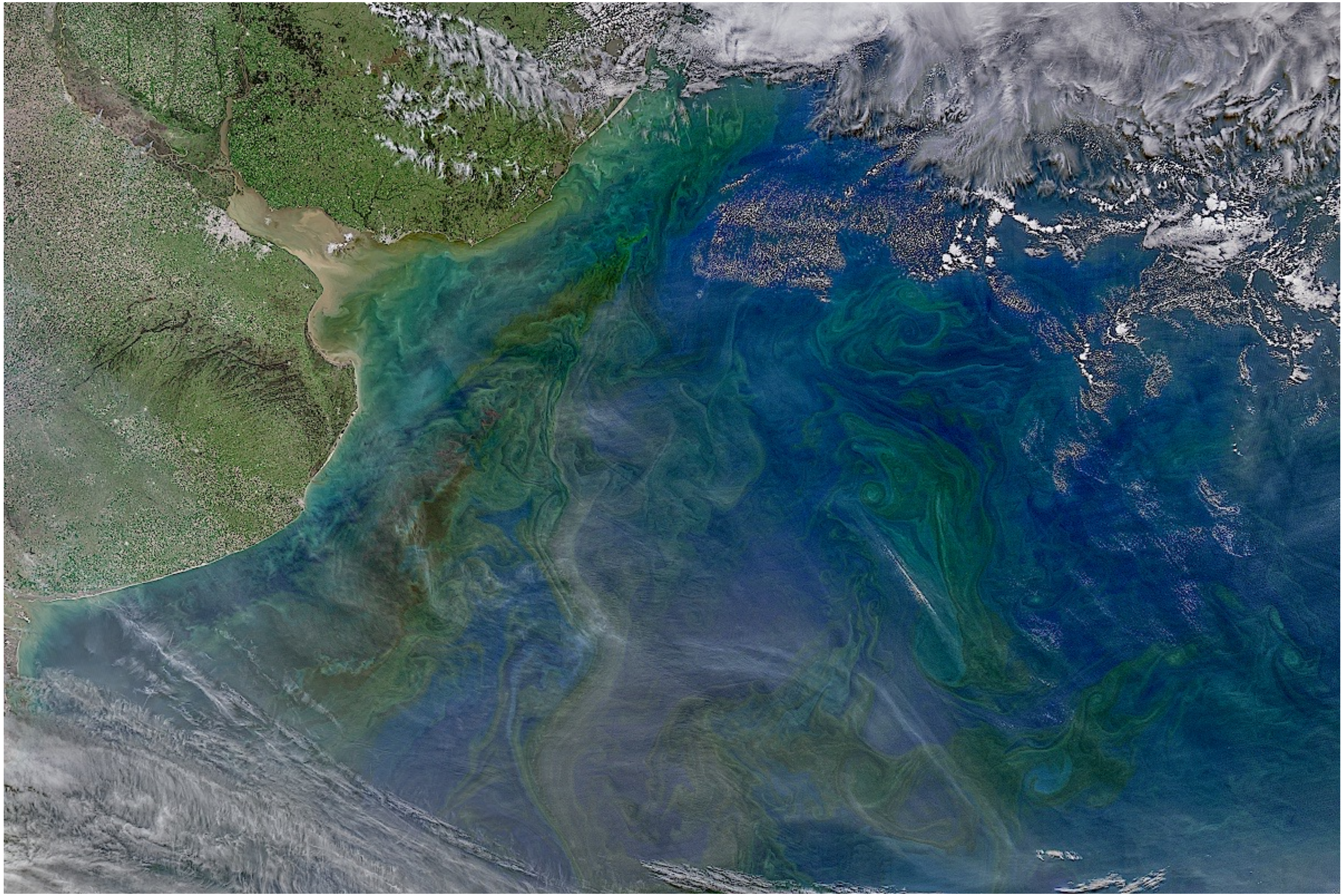
The color of the ocean is a function of light that is absorbed or scattered as a result of constituents in the water.

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



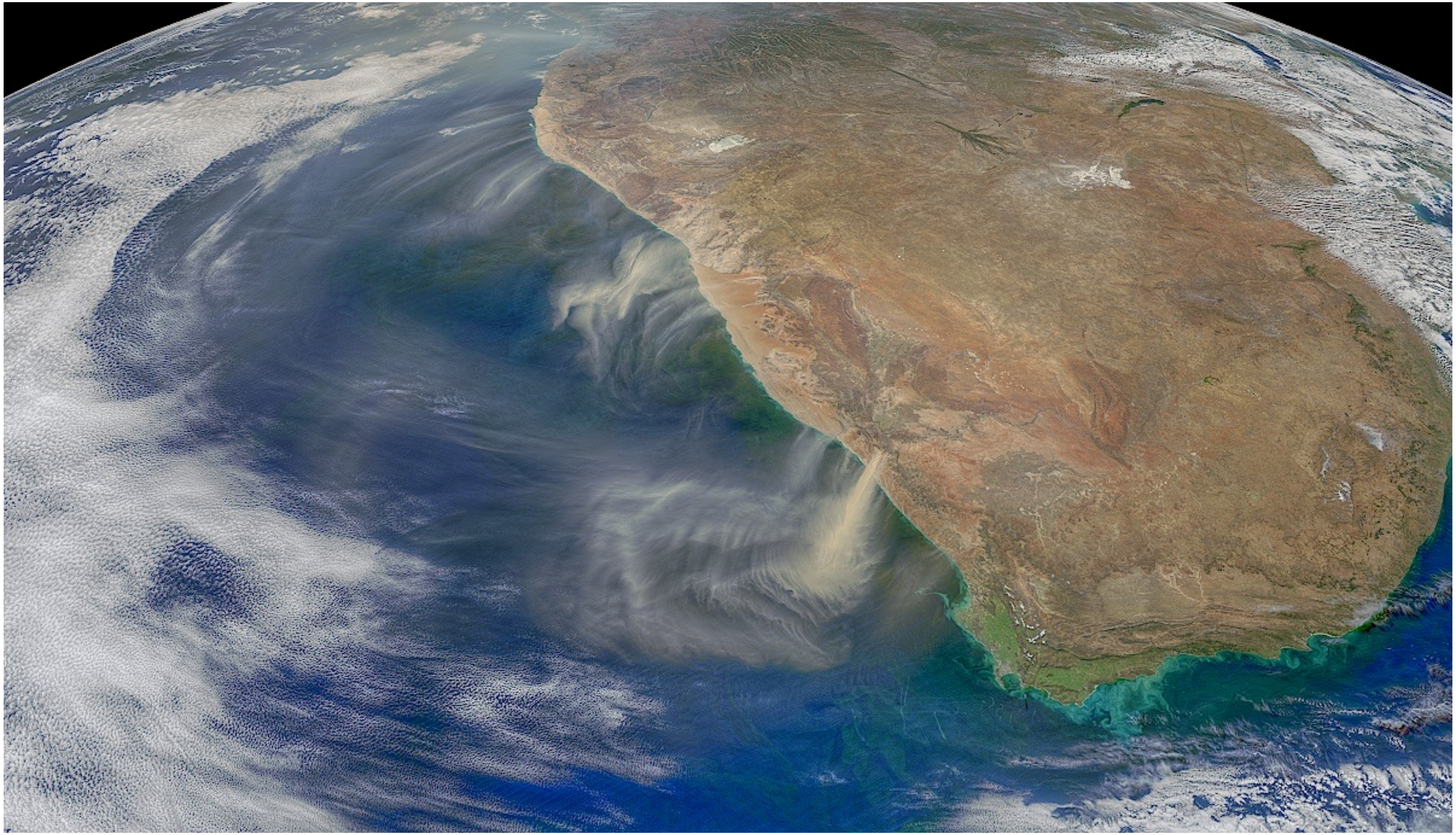


What do we observe from a spaceborne sensor?



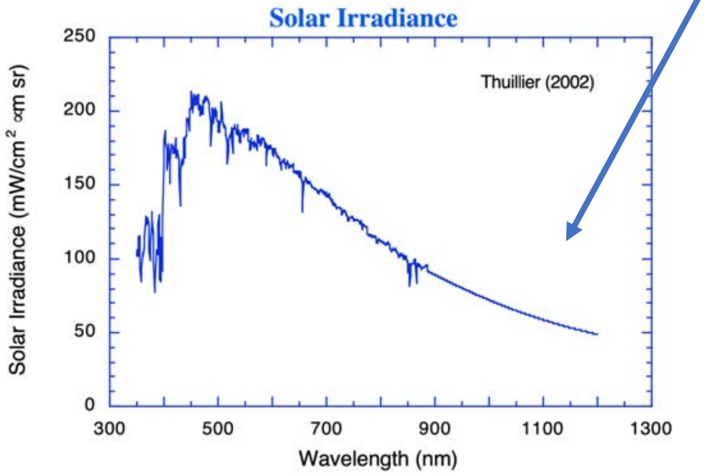
True color images from MODIS-Aqua - September 17, 2021

What do we observe from a spaceborne sensor?

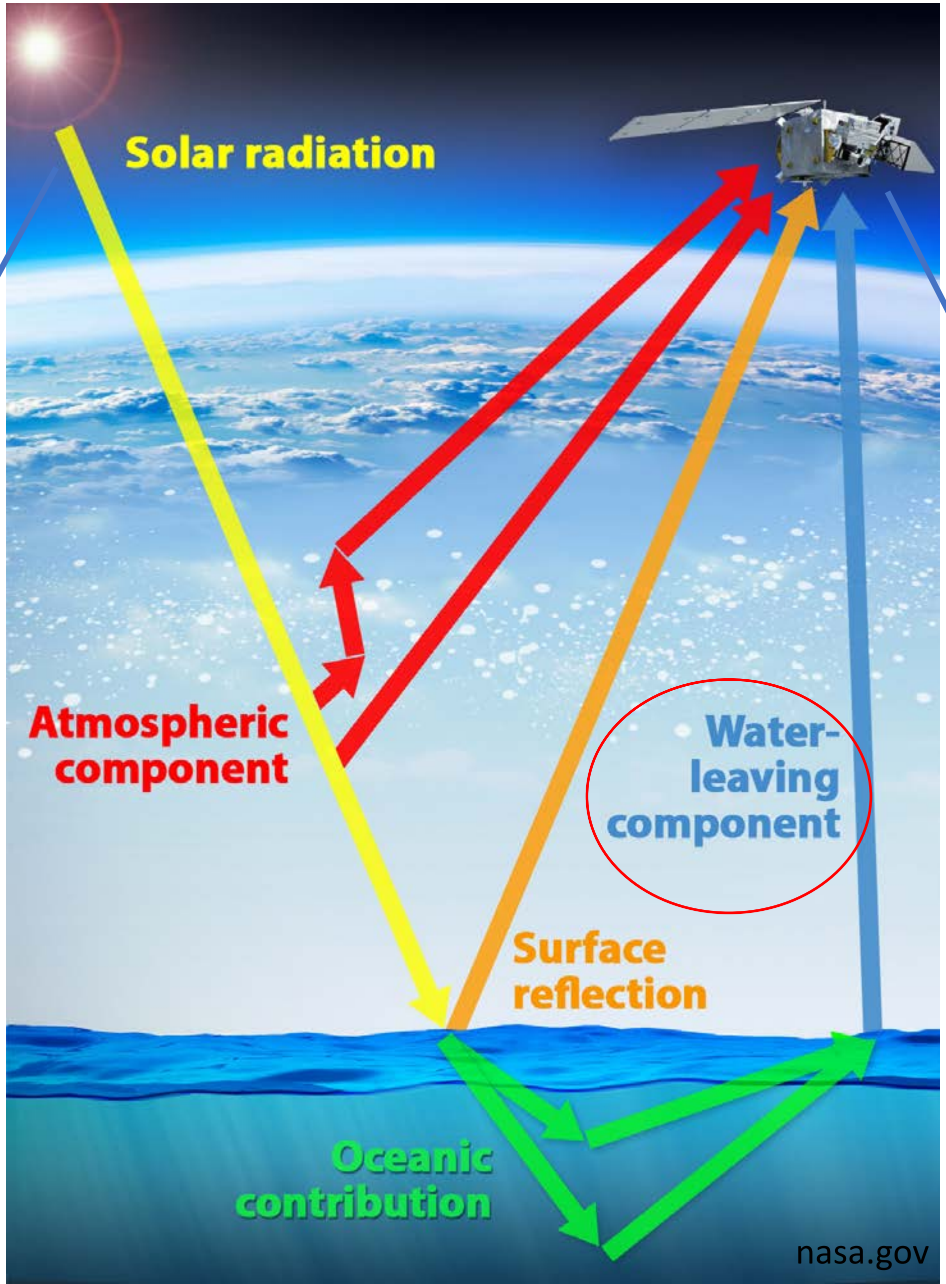


VIIRS—NPP - July 16, 2020

Ocean Color is a passive remote sensing technique

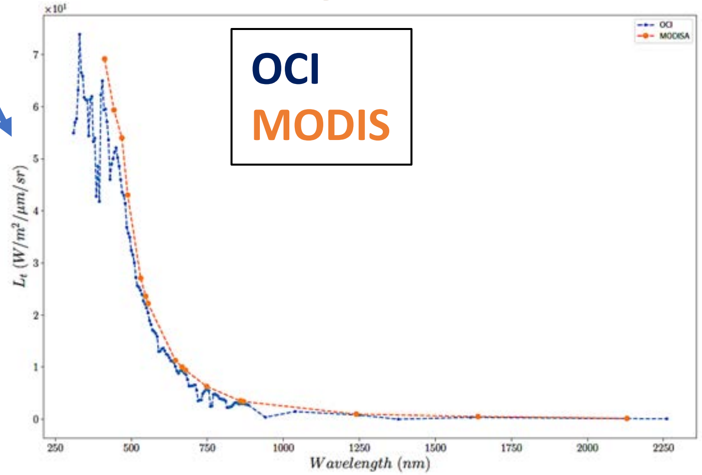


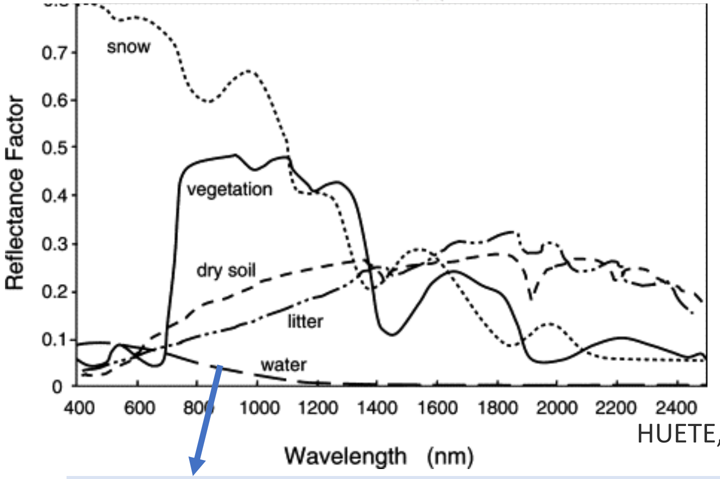
IOCCG



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

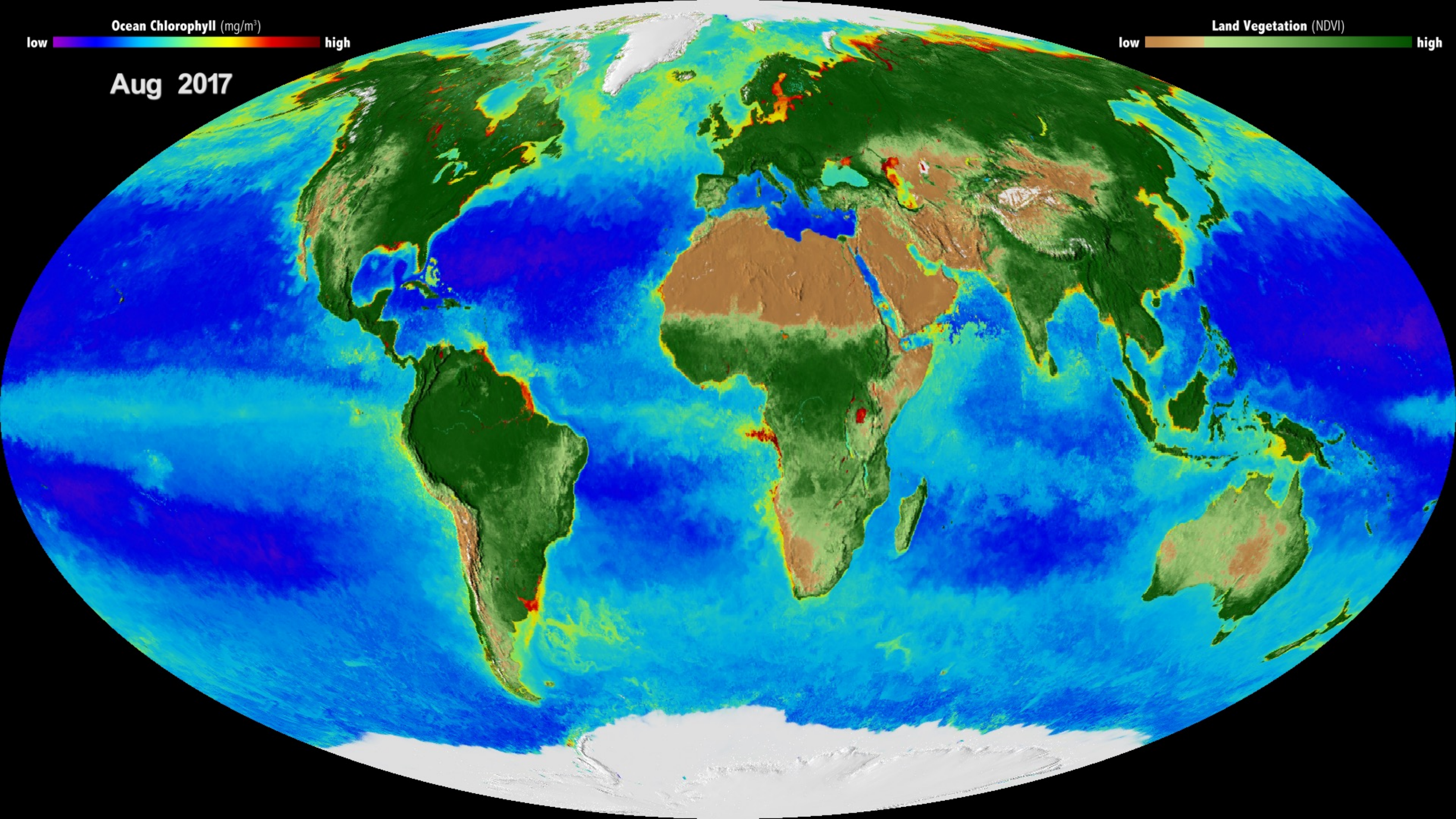
"Atmospheric correction"





HUETE, 2004

One scientist's noise is another's signal


Ocean Chlorophyll (mg/m³)
low
high
Land Vegetation (NDVI)
low
high
Aug 2017

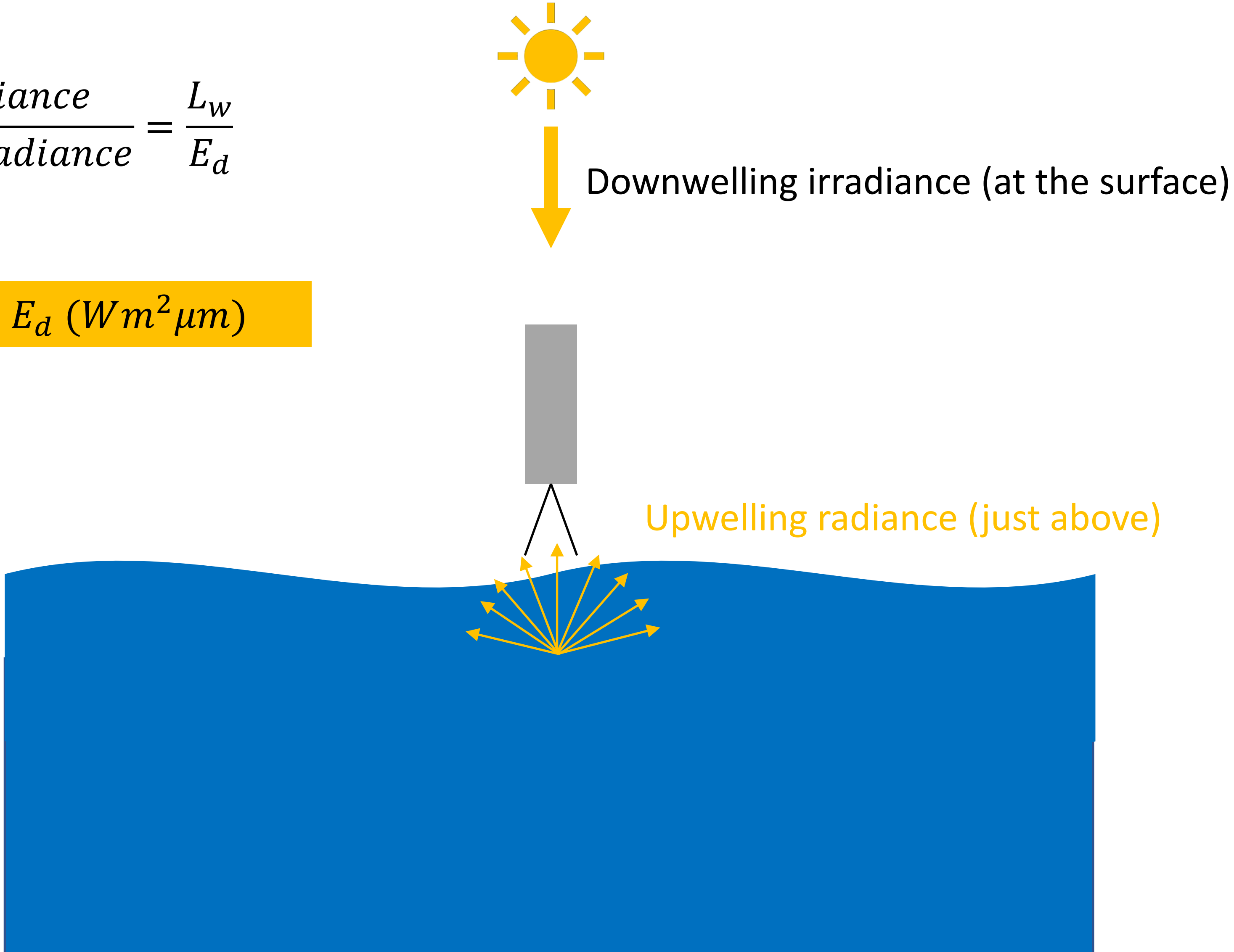
Remote sensing reflectance (R_{rs} ; sr^{-1})

$$R_{rs} = \frac{upwelling\ radiance}{downwelling\ irradiance} = \frac{L_w}{E_d}$$

$L_w\ (Wm^2\mu m\ sr^{-1})$

$E_d\ (Wm^2\mu m)$

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



Requirements for R_{rs} ($\rho_w = \pi R_{rs}$)

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%

these are required for mission success & drive OCI design

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

Atmospheric Correction using OCI alone

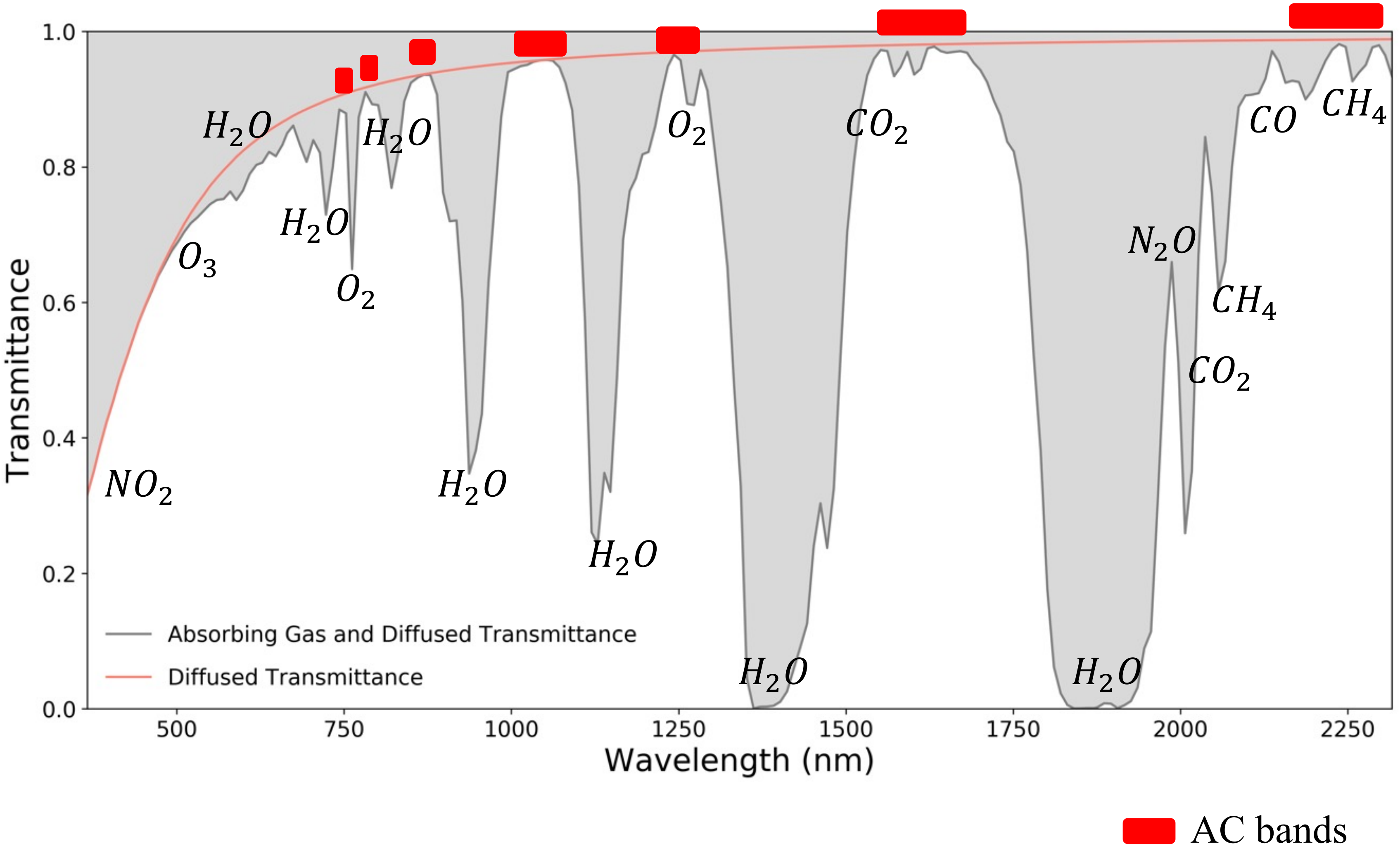
*Better characterization of aerosols using MAP

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).

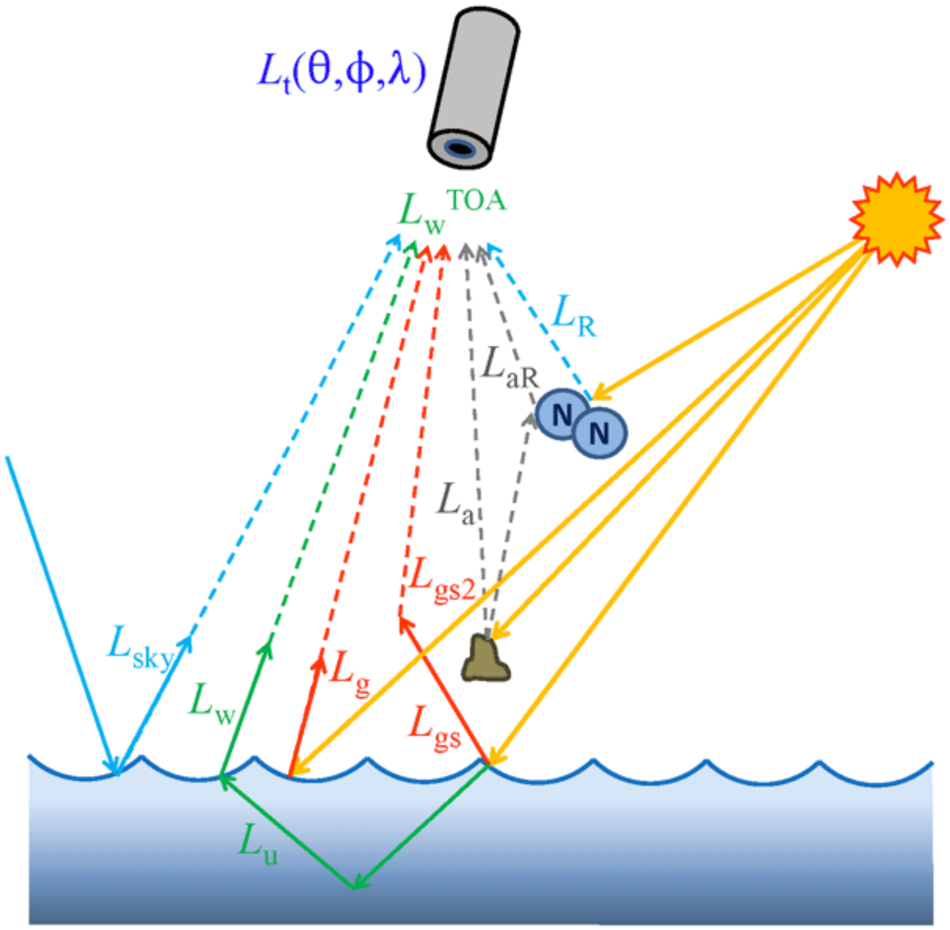
Atmospheric Correction

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

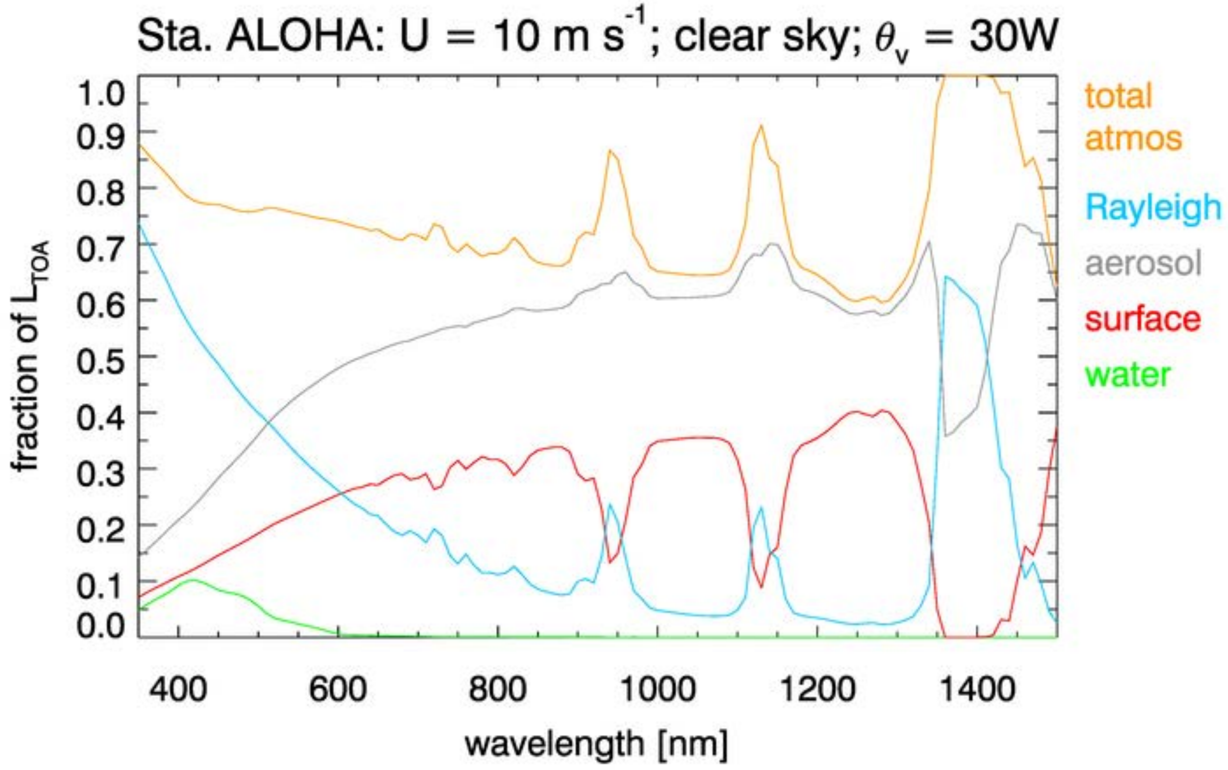
$$L_t(\lambda) = \left(L_r(\lambda) + L_a(\lambda) + L_{ra}(\lambda) + t(\lambda)L_f(\lambda) + T(\lambda)L_g(\lambda) + t(\lambda)L_w(\lambda)\right) \times T_g(\lambda)$$



Formulation



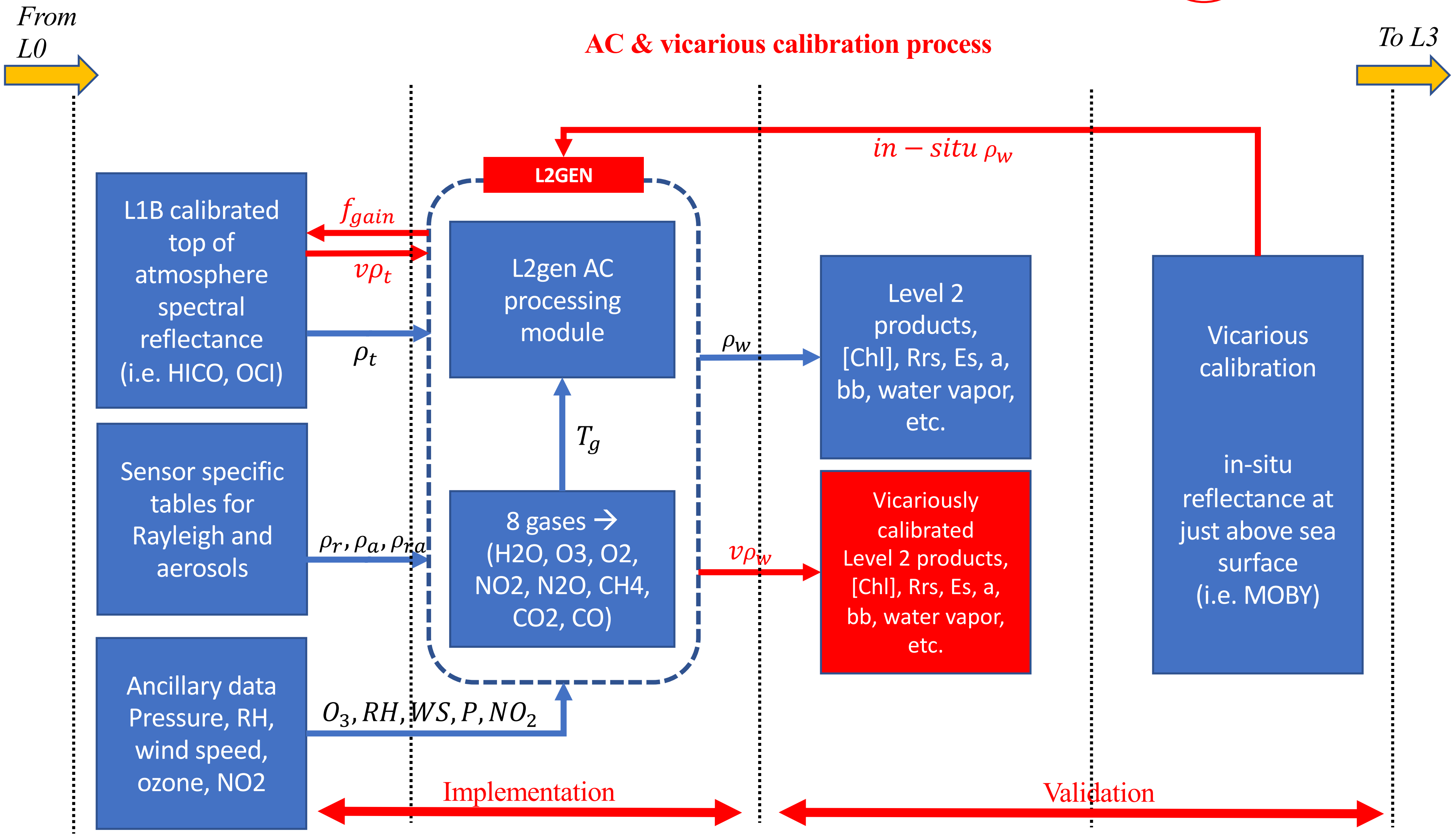
Mobley et al., 2016



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

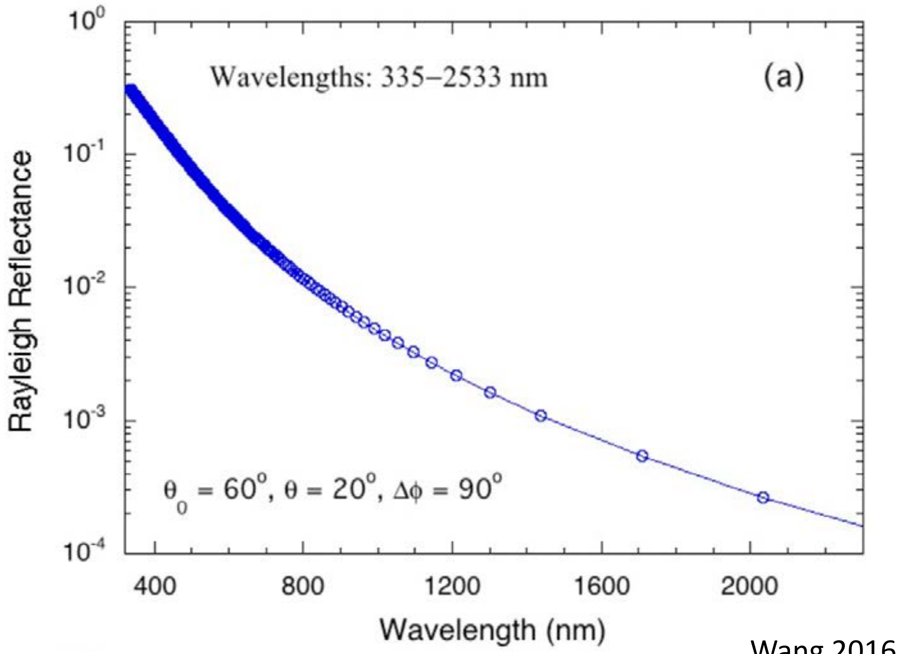
NASA's operational AC algorithm

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

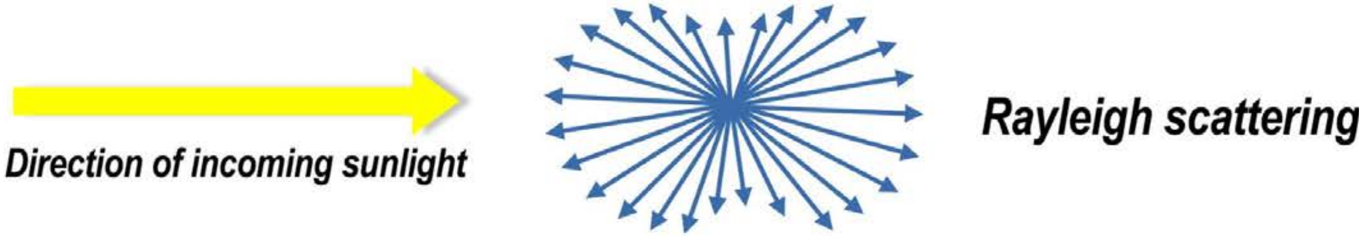


Rayleigh scattering $L_r(\lambda)$

- 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.

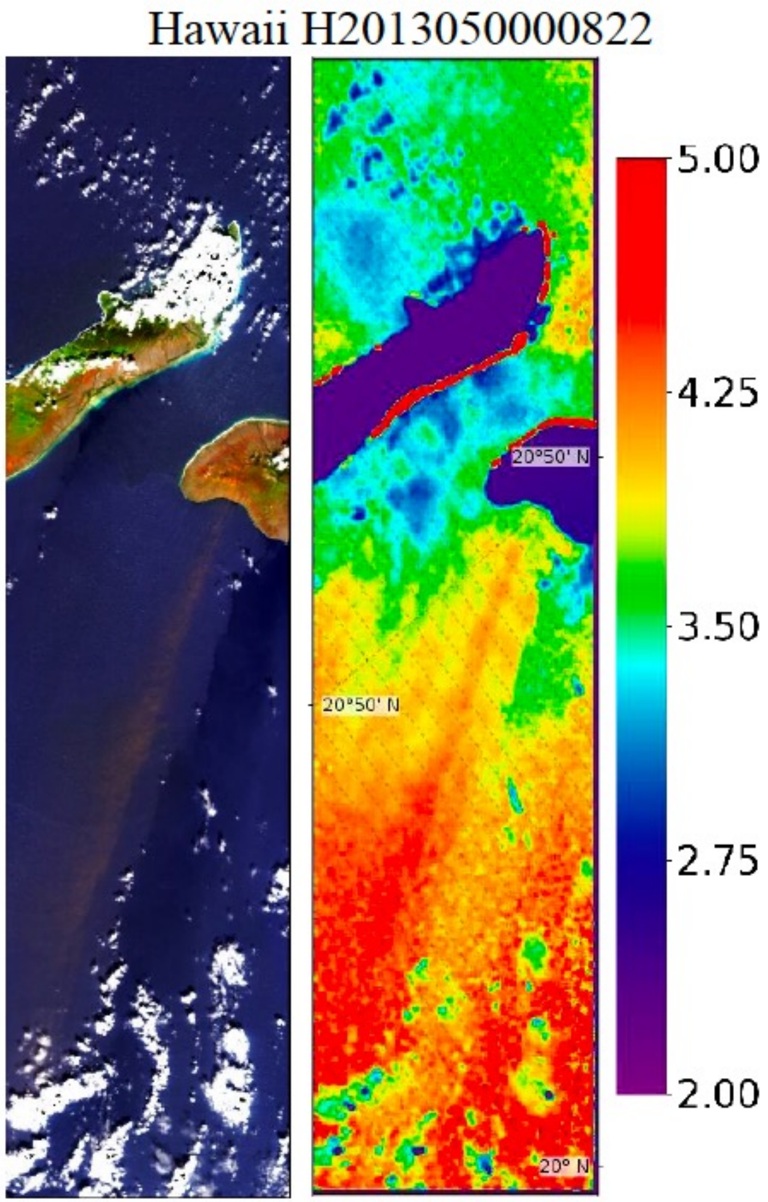


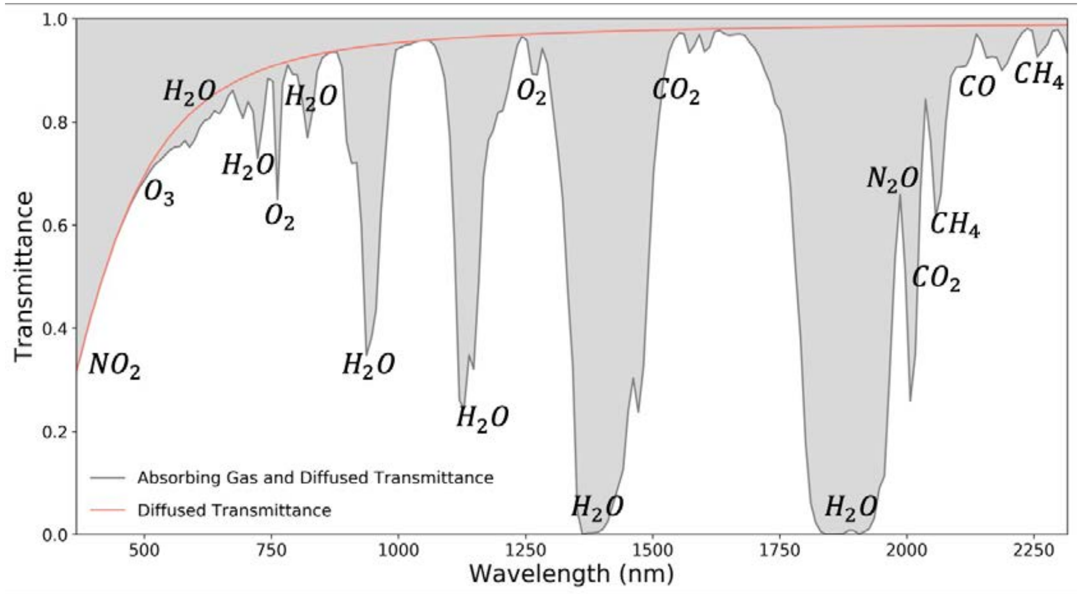
Wang 2016

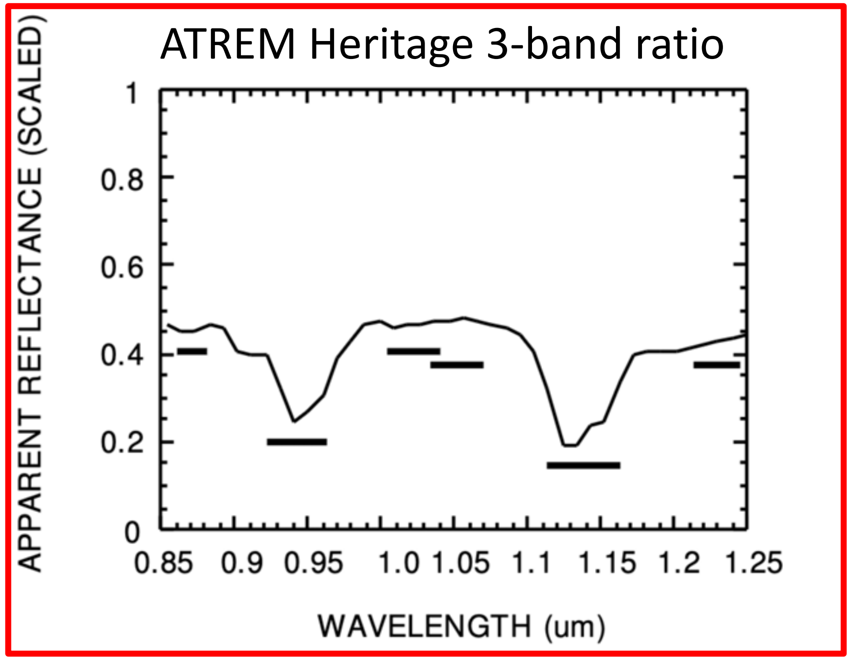


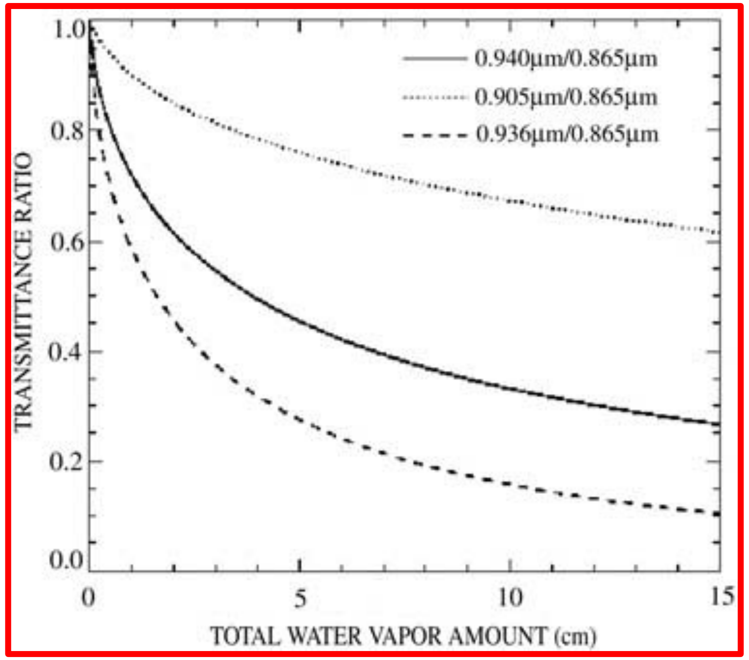
$$L_t(\lambda) = \left(L_r(\lambda) + L_a(\lambda) + L_{ra}(\lambda) + t(\lambda)L_f(\lambda) + T(\lambda)L_g(\lambda) + t(\lambda)L_w(\lambda)\right) \times T_g(\lambda)$$

Gas absorption correction $T_g(\lambda)$





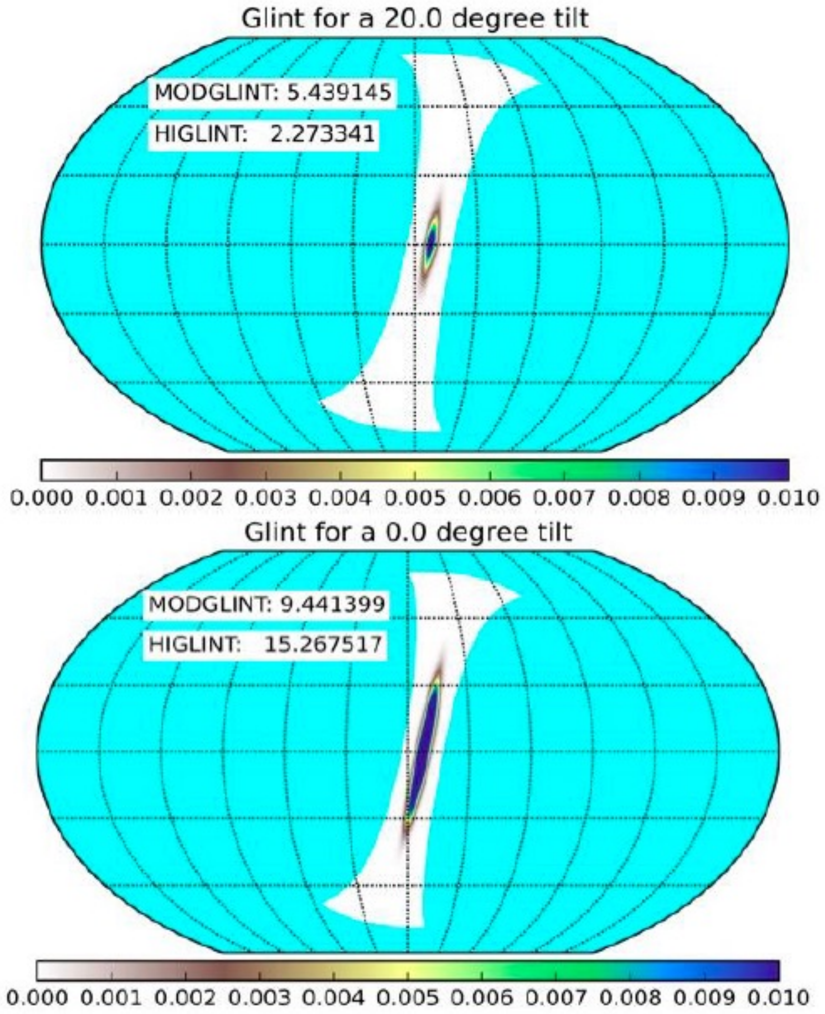


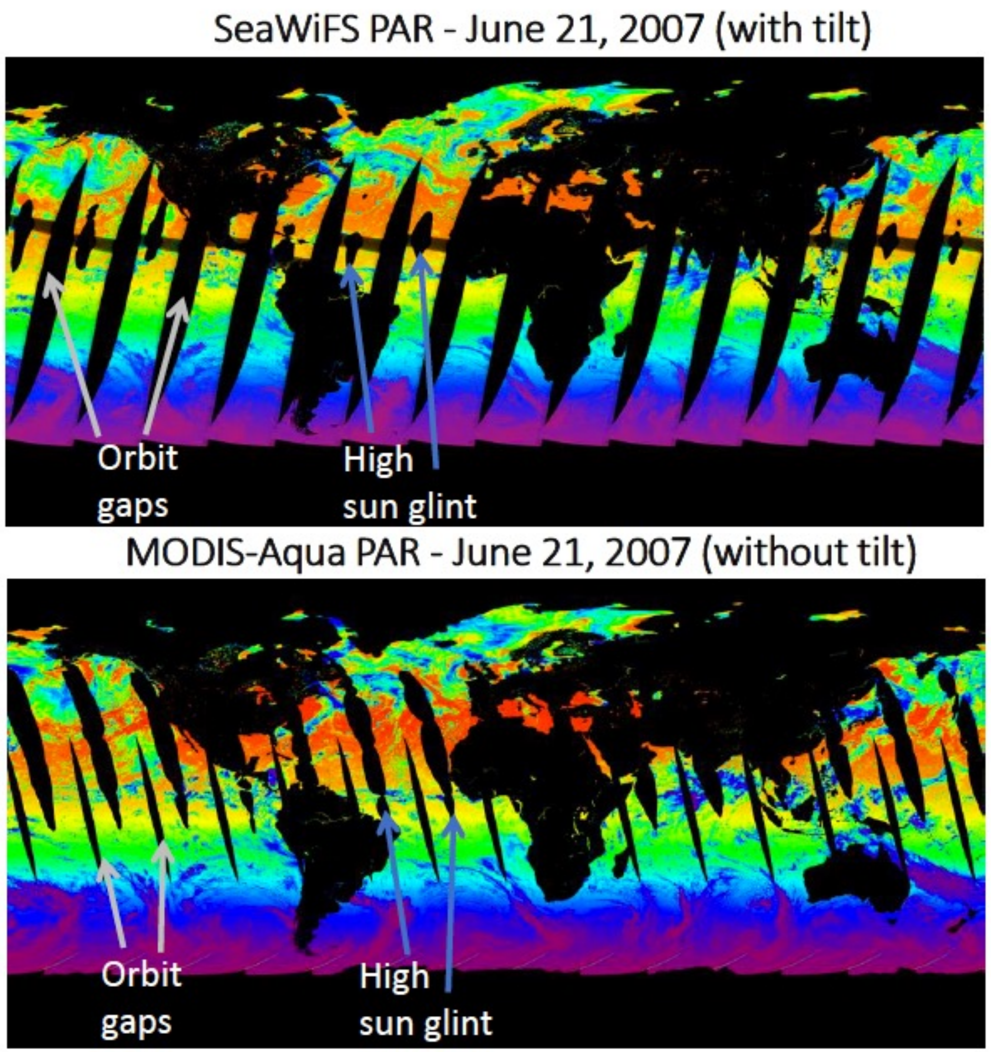


Direct sun glint $\boldsymbol{T(\lambda)L_g(\lambda)}$

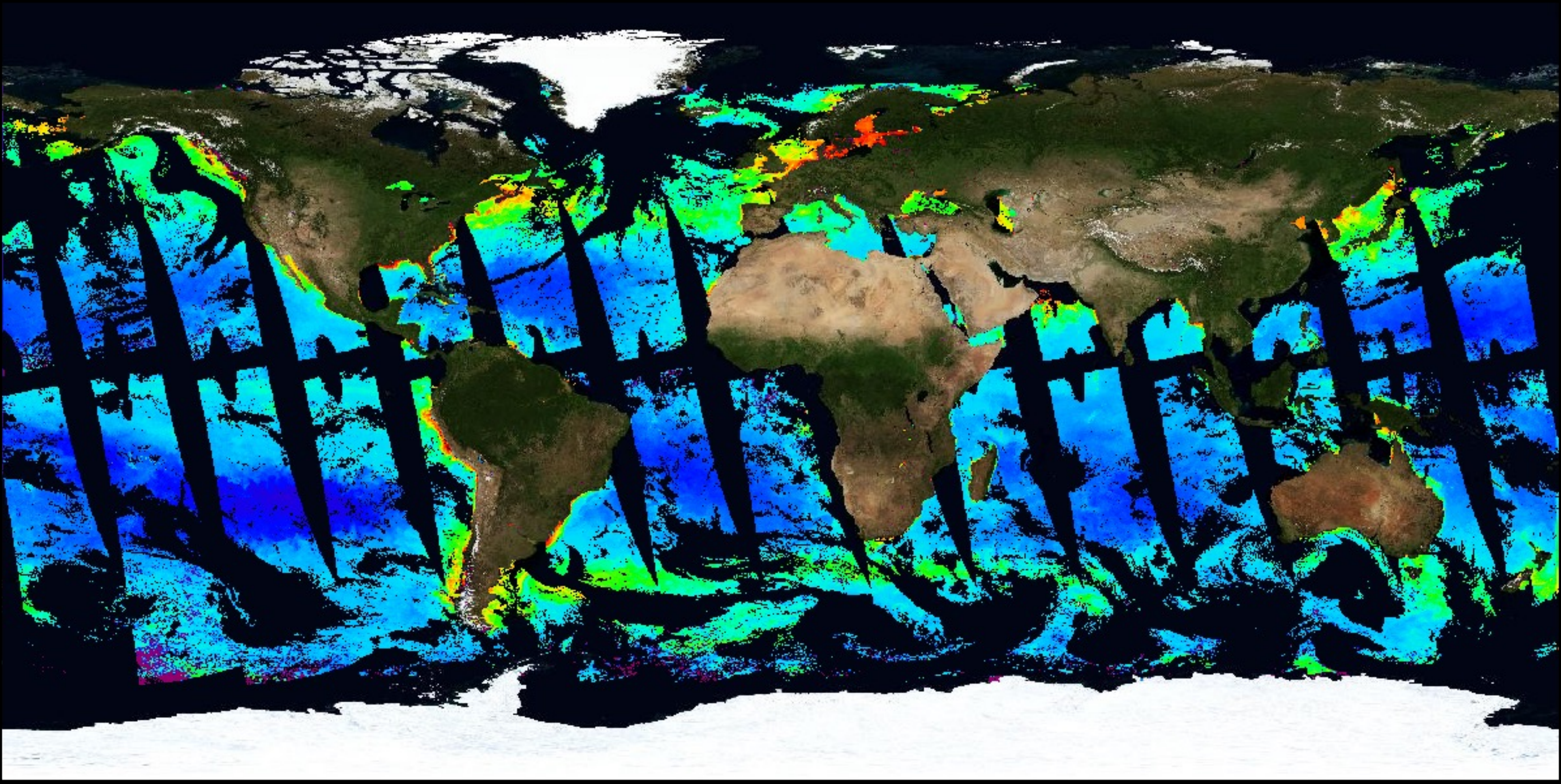
OCI tilt to avoid glint and increase coverage

OCI is tilted 20˚ to avoid glint





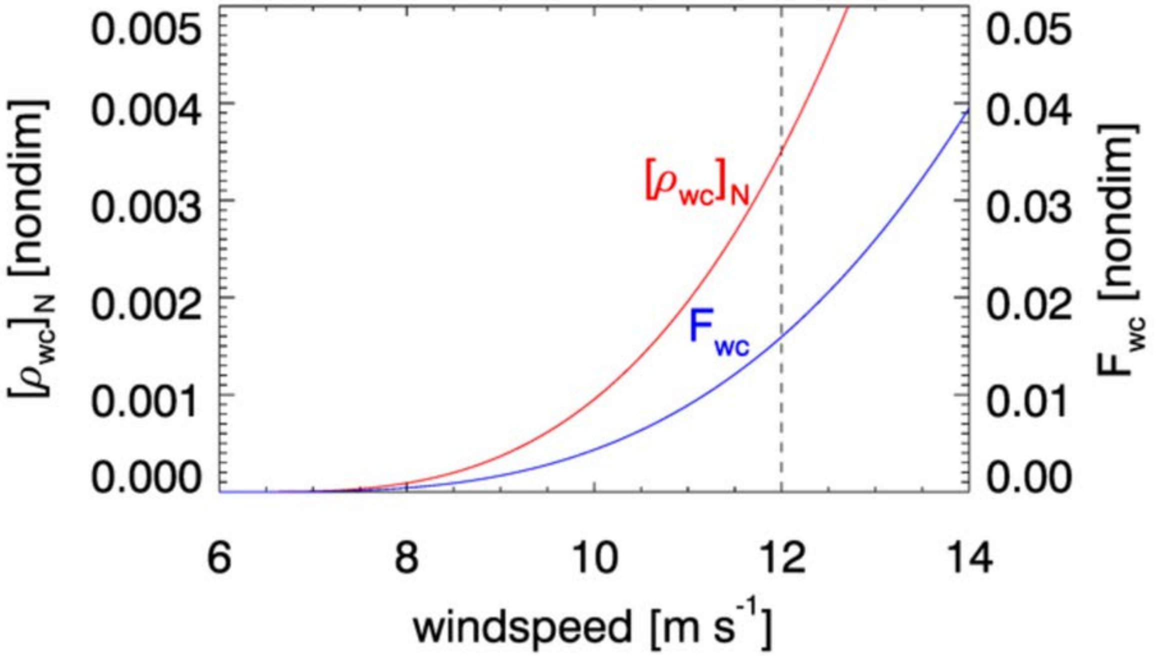
PAR = Photosynthetically Available Radiation



White caps $t(\lambda)L_f(\lambda)$

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

$$[\rho_{\mathrm{wc}}]_{\mathrm{N}}(\lambda) = a_{\mathrm{wc}}(\lambda) \times 0.22 \times F_{\mathrm{wc}} = a_{\mathrm{wc}}(\lambda) \times 1.925 \times 10^{-5}(U_{10} - 6.33)^3 .$$



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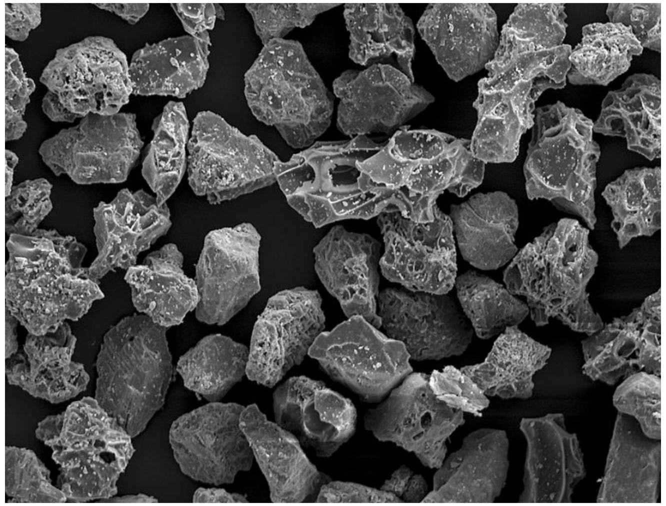
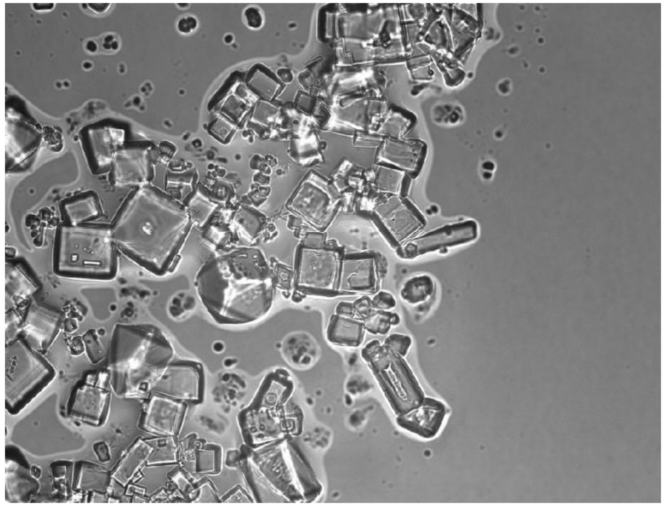
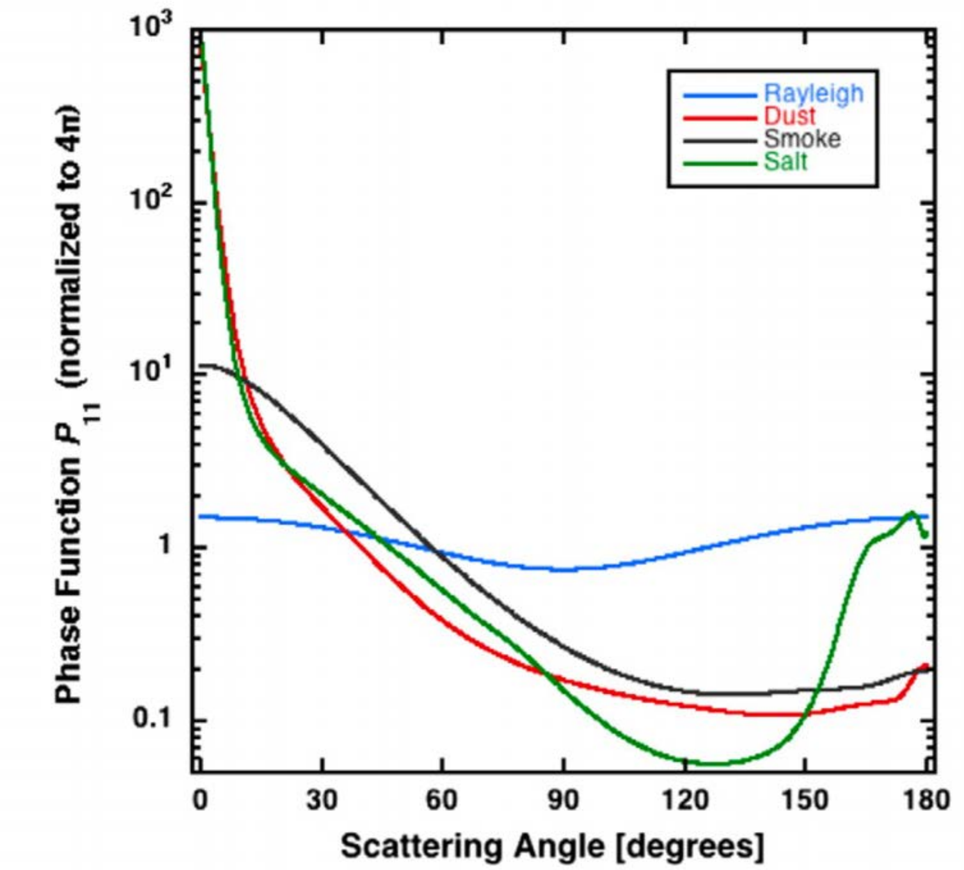
Aerosols challenge

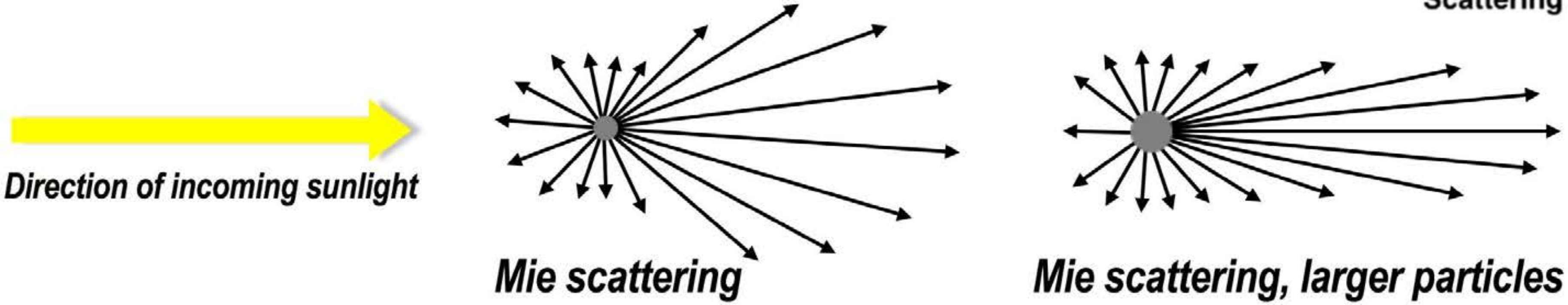
- ✓Complex morphology.
- ✓Chemical composition.
- ✓Size distribution.

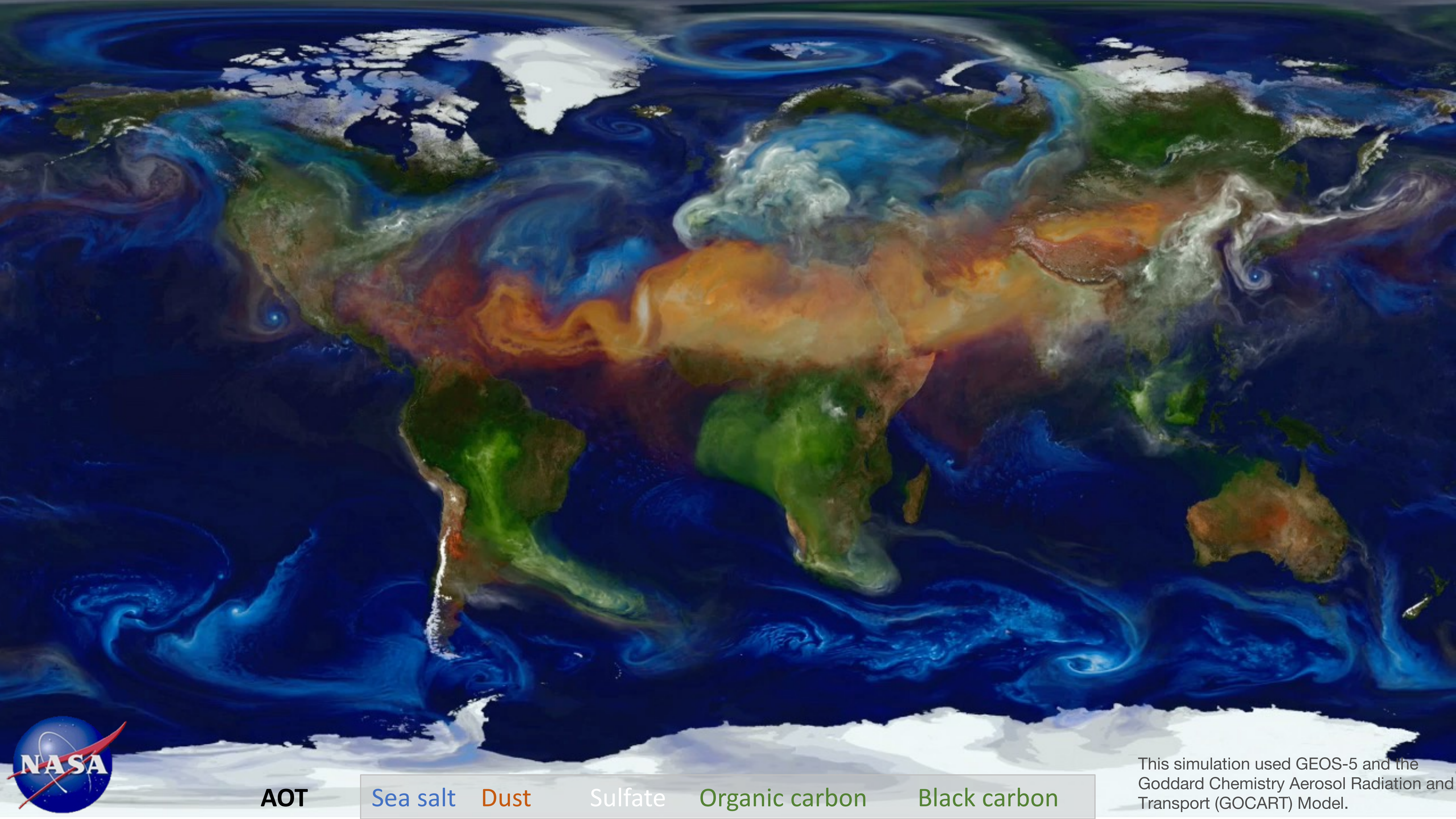






Kokhanovsky et al., 2015





This simulation used GEOS-5 and the Goddard Chemistry Aerosol Radiation and Transport (GOCART) Model.

Aerosol microphysical model

80 aerosol models (10 fine mode fractions x 8 relative humidities)

Ahmad et al., 2010

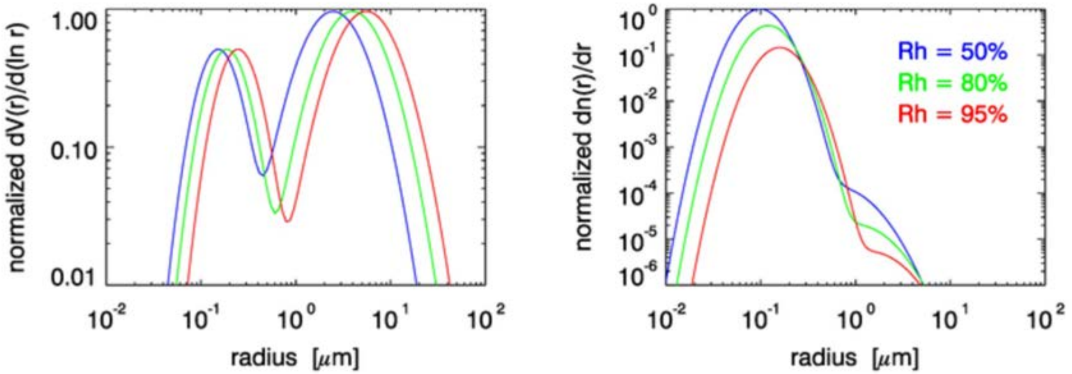
Table 1. Complex Refractive Index Values for Different Constituents of the Fine and Coarse Mode Aerosols for SeaWiFS Sensor at Relative Humidity Rh = 0 (SF79).

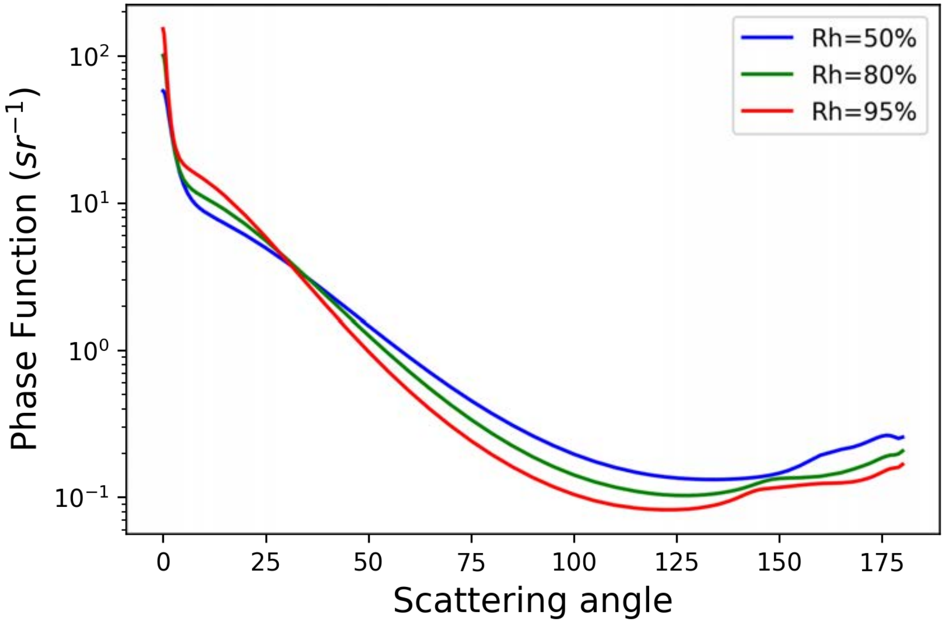
Wavelength (nm)	Water-Soluble	Dustlike	Sea Salt	Soot	Water
412	1.530 – 0.0050i	1.530 – 0.0080i	1.500 – 0.0000i	1.750 – 0.4586i	1.338 – 0.0000i
443	1.530 – 0.0050i	1.530 – 0.0080i	1.500 – 0.0000i	1.750 – 0.4551i	1.337 – 0.0000i
490	1.530 – 0.0050i	1.530 – 0.0080i	1.500 – 0.0000i	1.750 – 0.4500i	1.335 – 0.0000i
510	1.530 – 0.0050i	1.530 – 0.0080i	1.500 – 0.0000i	1.750 – 0.4500i	1.334 – 0.0000i
555	1.530 – 0.0060i	1.530 – 0.0080i	1.499 – 0.0000i	1.750 – 0.4394i	1.333 – 0.0000i
670	1.530 – 0.0066i	1.530 – 0.0080i	1.490 – 0.0000i	1.750 – 0.4300i	1.331 – 0.0000i
765	1.526 – 0.0091i	1.526 – 0.0080i	1.486 – 0.0000i	1.750 – 0.4300i	1.330 – 0.0000i
865	1.520 – 0.0121i	1.520 – 0.0080i	1.480 – 0.0000i	1.750 – 0.4303i	1.329 – 0.0000i

Table 4. Modal Radii (r_{vf}, r_{vc}), Standard Deviations (σ_f, σ_c), and Ratios of Wet-to-Dry Aerosol Radius ($r_{vf}/r_{ovf}, r_{vc}/r_{ovc}$) for Eight Values of Relative Humidity Used in This Study[a]

Rh	r_{vf}	σ_f	r_{vc}	σ_c	r_{vf}/r_{ovf}	r_{vc}/r_{ovc}
0.30	0.150	0.437	2.441	0.672	1.006	1.009
0.50	0.152	0.437	2.477	0.672	1.019	1.024
0.70	0.158	0.437	2.927	0.672	1.063	1.210
0.75	0.167	0.437	3.481	0.672	1.118	1.439
0.80	0.187	0.437	3.966	0.672	1.255	1.639
0.85	0.204	0.437	4.243	0.672	1.371	1.753
0.90	0.221	0.437	4.638	0.672	1.486	1.917
0.95	0.246	0.437	5.549	0.672	1.648	2.293

[a]The subscripts v, f, and c, respectively, refer to volume space, fine mode, and coarse mode of the aerosols





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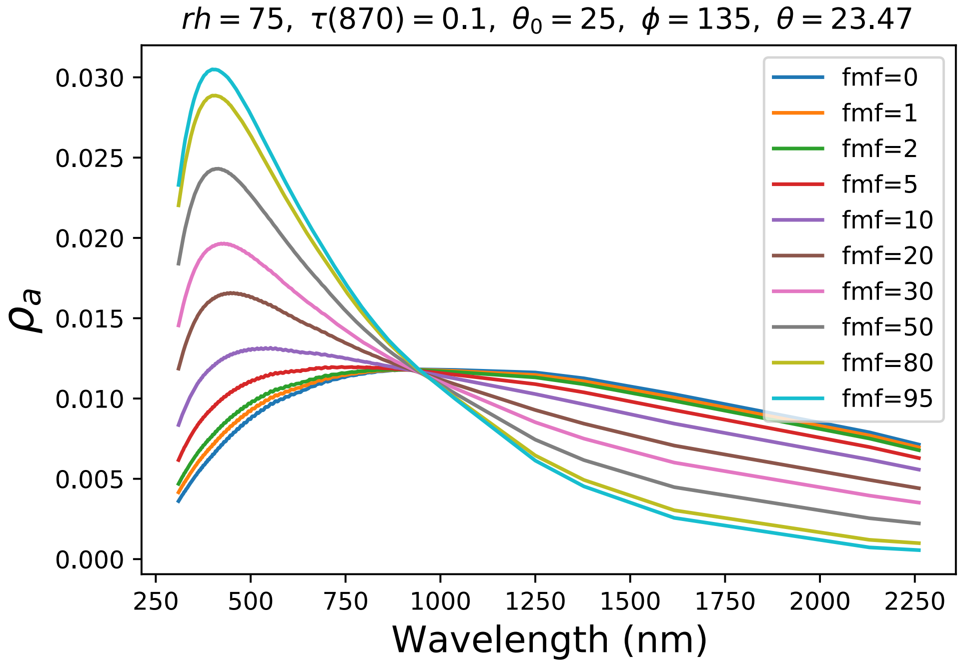
Aerosol LUTs $L_a(\lambda) + L_{ra}(\lambda)$

- To perform the AC, we need to generate aerosol LUTs.
- Perform multidimensional linear interpolation for each pixel of the granule.
- Dimensions of aerosol reflectance (ρ_a) LUT:

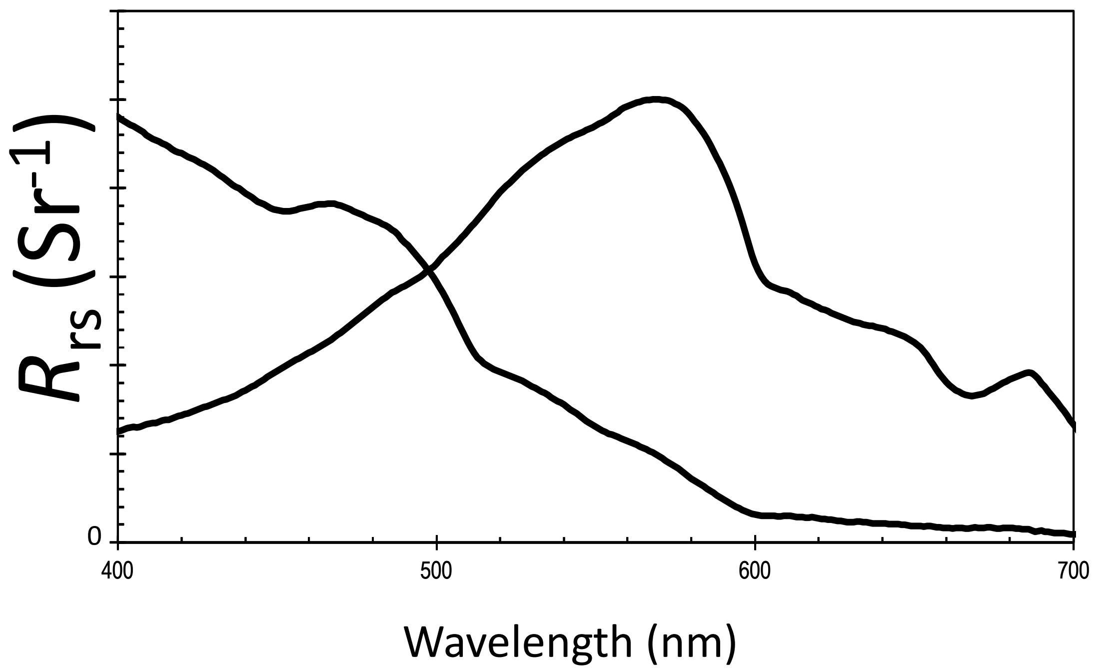
relative humidity (rh): 8
fine-mode fractions (fmf): 10
optical depth ($\boldsymbol{\tau}$): 9
*Hyperspectral → wavelengths (λ): 239
solar zenith (θ_0): 33
relative azimuth (φ): 19
sensor zenith (θ): 35

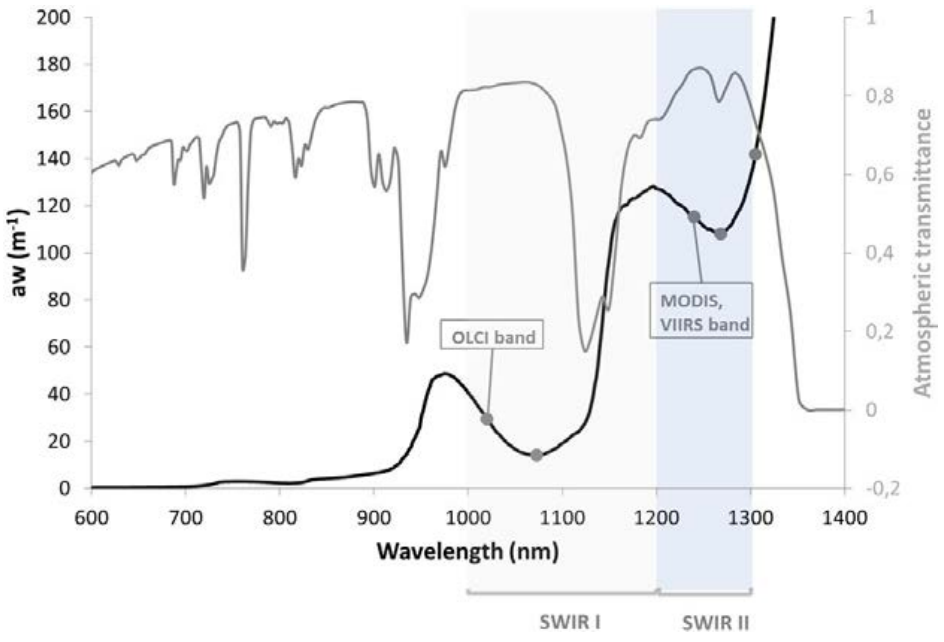
~3.8 billion data point!



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

Black pixel assumption for aerosol correction

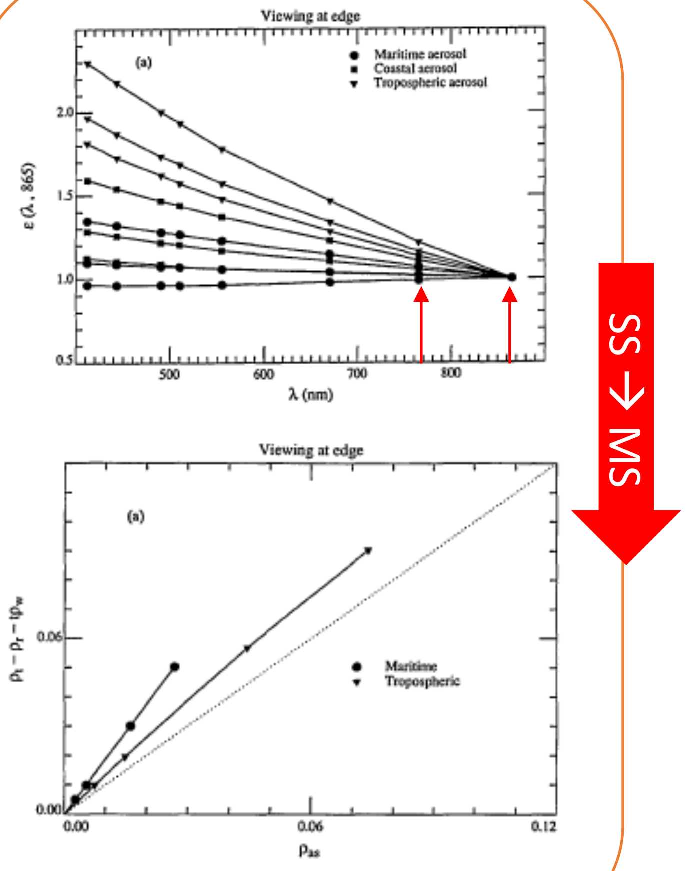




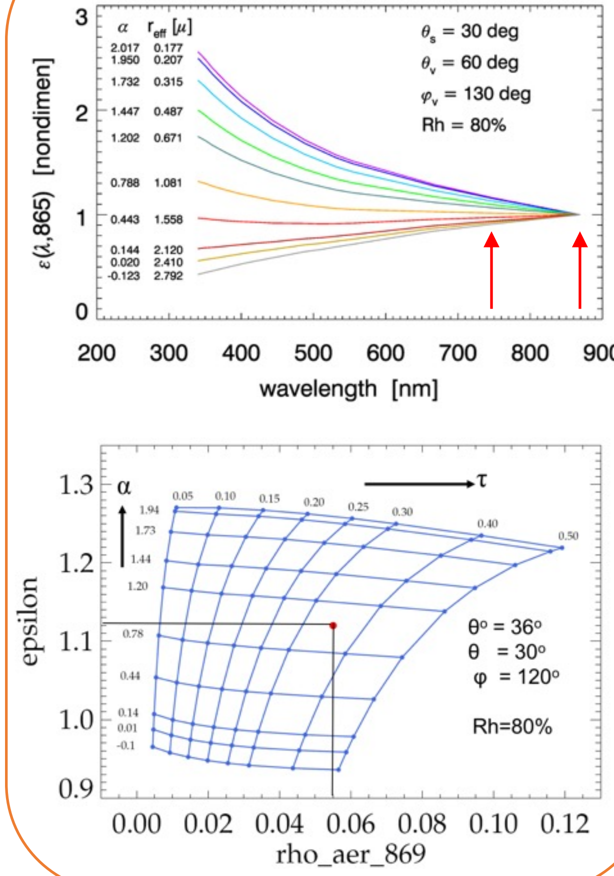
NASA's operational AC algorithm with focus on the aerosols correction

- Heritage and recent advancements in AC algorithms:

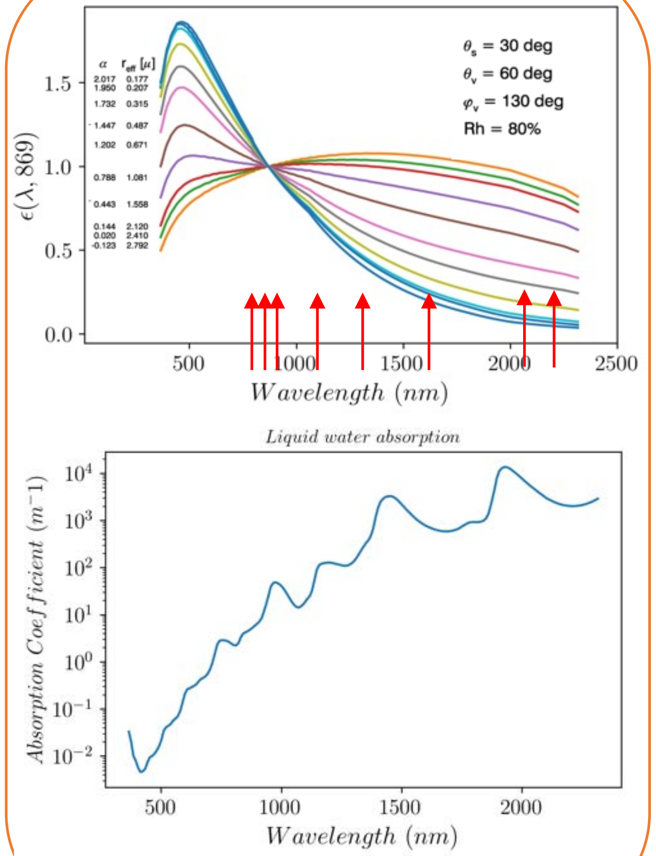
Gordon and Wang, 1994



MSEPS
Ahmad et al., 2010



MBAC
Ibrahim et al., 2019



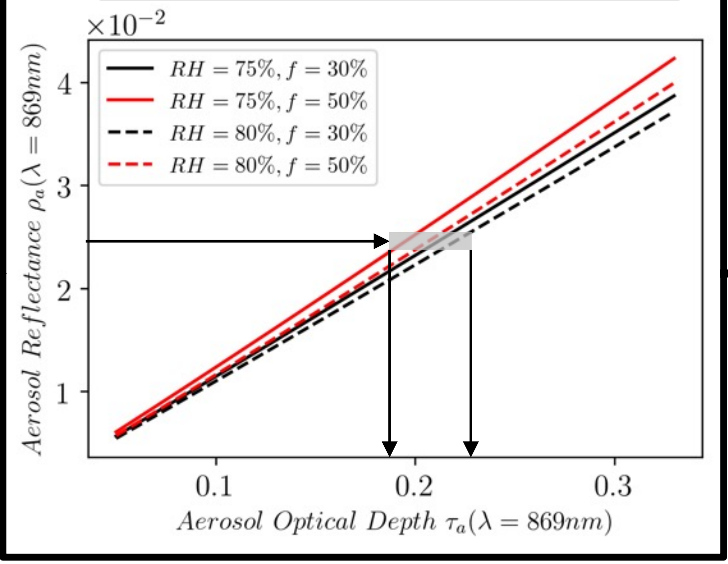
Multi-band Atmospheric Correction (MBAC)

TOA radiance Lt

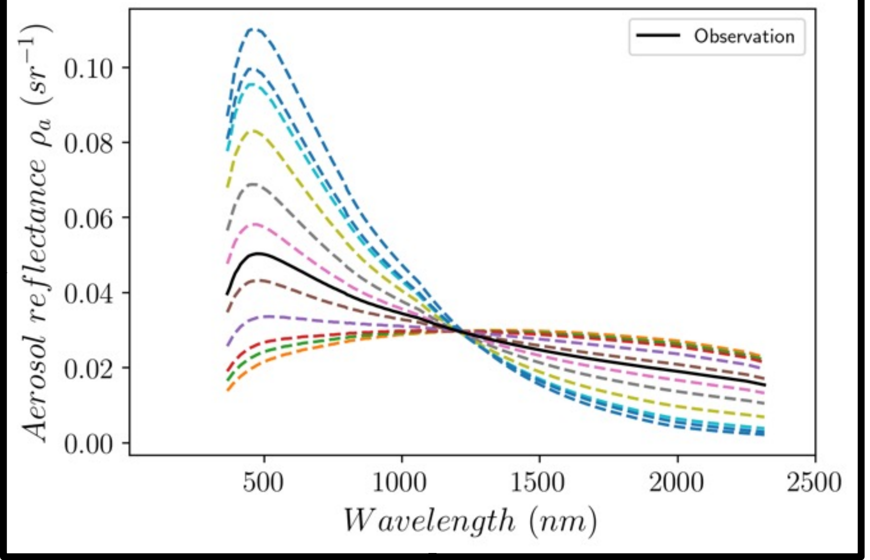
Rayleigh, gas, and glint correction

L_{rgc}

Estimate the optical depth at the longest high radiometric quality band



Estimate the aerosol spectral reflectance for a set of models



$\nabla\chi^2$ minimization

$$\chi^2(RH,f) = \frac{1}{DOF} \times \sum_{\lambda=\lambda_s}^{\lambda_l} \frac{[\rho_{obs}(\lambda) - \rho_a(\lambda, RH, f)]^2}{\sigma^2(\lambda)} \times SW(\lambda)$$

Average best models, calculate transmittances

R_{rs}, τ_a, Ångström

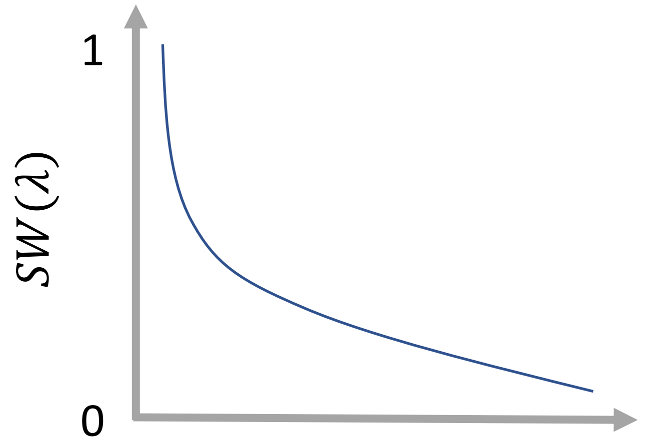
Ibrahim et al., 2019

AC over turbid waters

- 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.

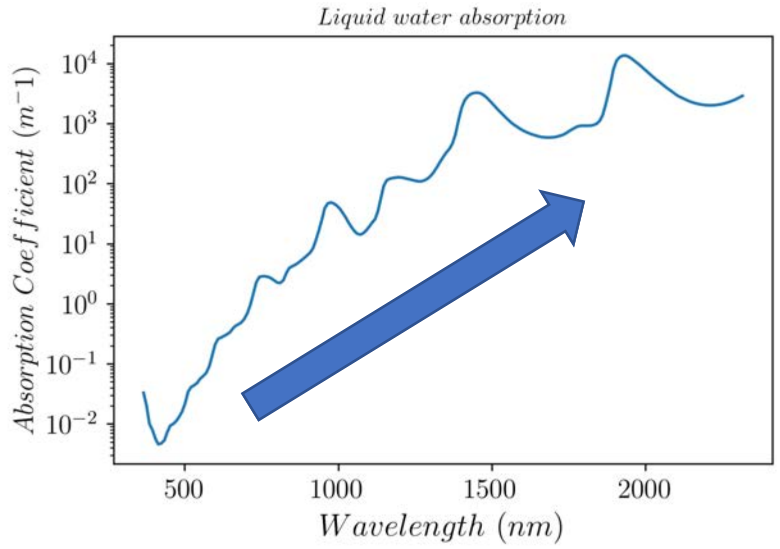
Sensor/ Wavelength (nm)								
MODIS	748	859	869		1240	1640	2130	
VIIRS	746	868			1238	1604		2258
PACE-OCI	750	860	870	1038	1250	1615	2130	2260

- The adaptive spectral weight for each band depends on the number of iterations in the NIR algorithm. More iterations means 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).



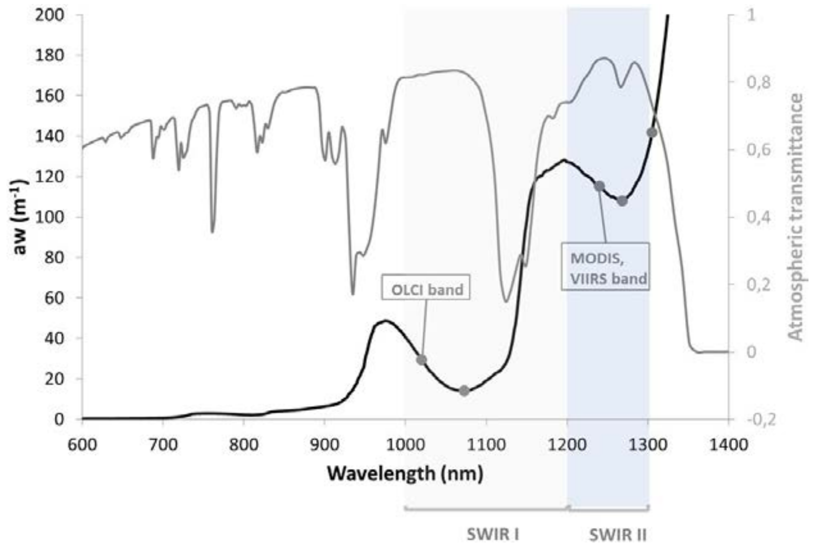
NIR iterations (Bailey et al., 2010)

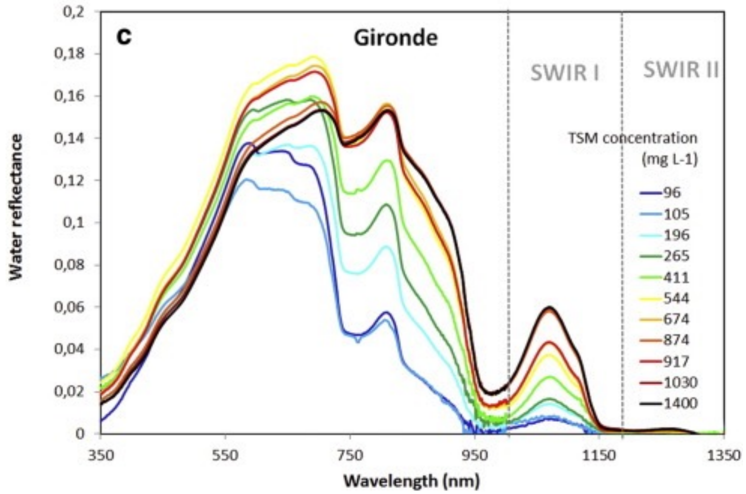
$$\chi^2(RH, f) = \frac{1}{DOF} \times \sum_{\lambda=\lambda_s}^{\lambda_l} \frac{[\rho_{obs}(\lambda) - \rho_a(\lambda, RH, f)]^2}{\sigma^2(\lambda)} \times SW(\lambda)$$

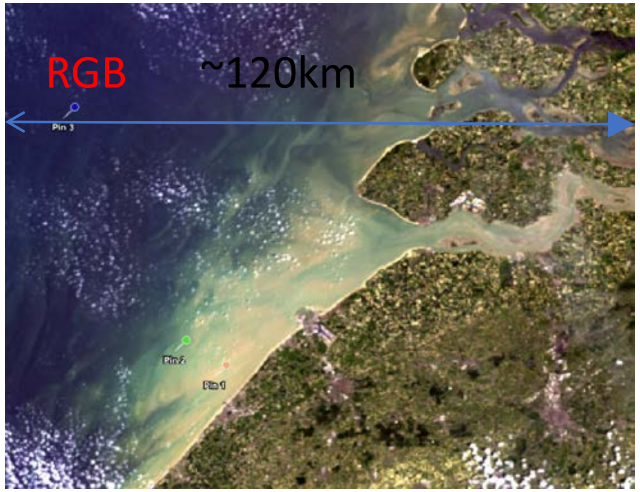


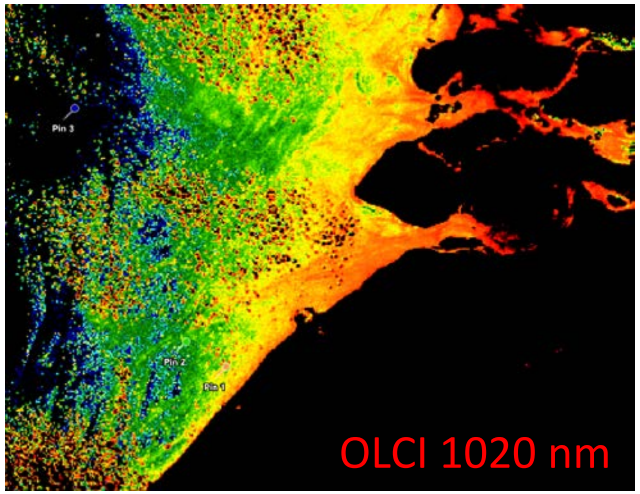
Application and benefits of OCI SWIR channels

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



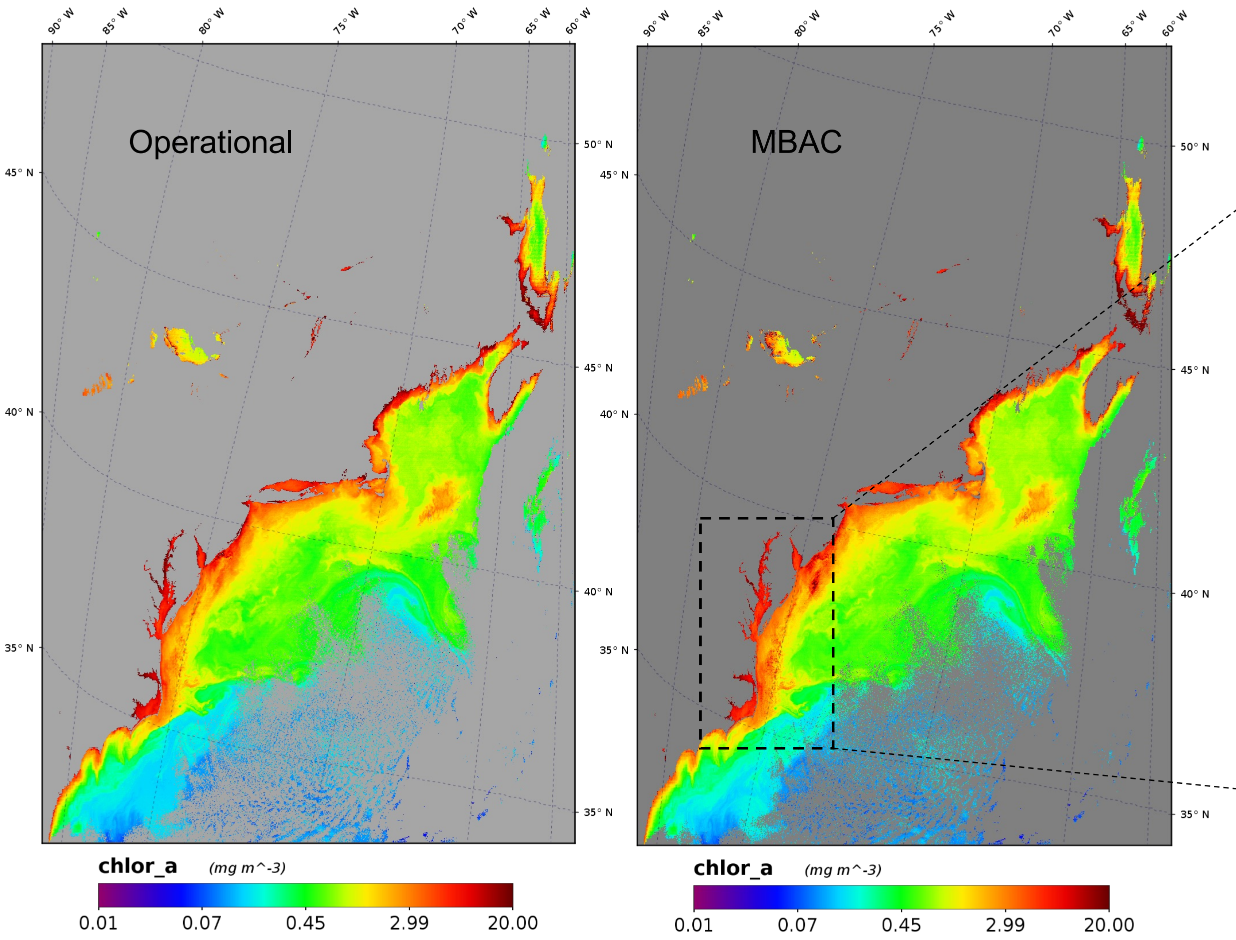


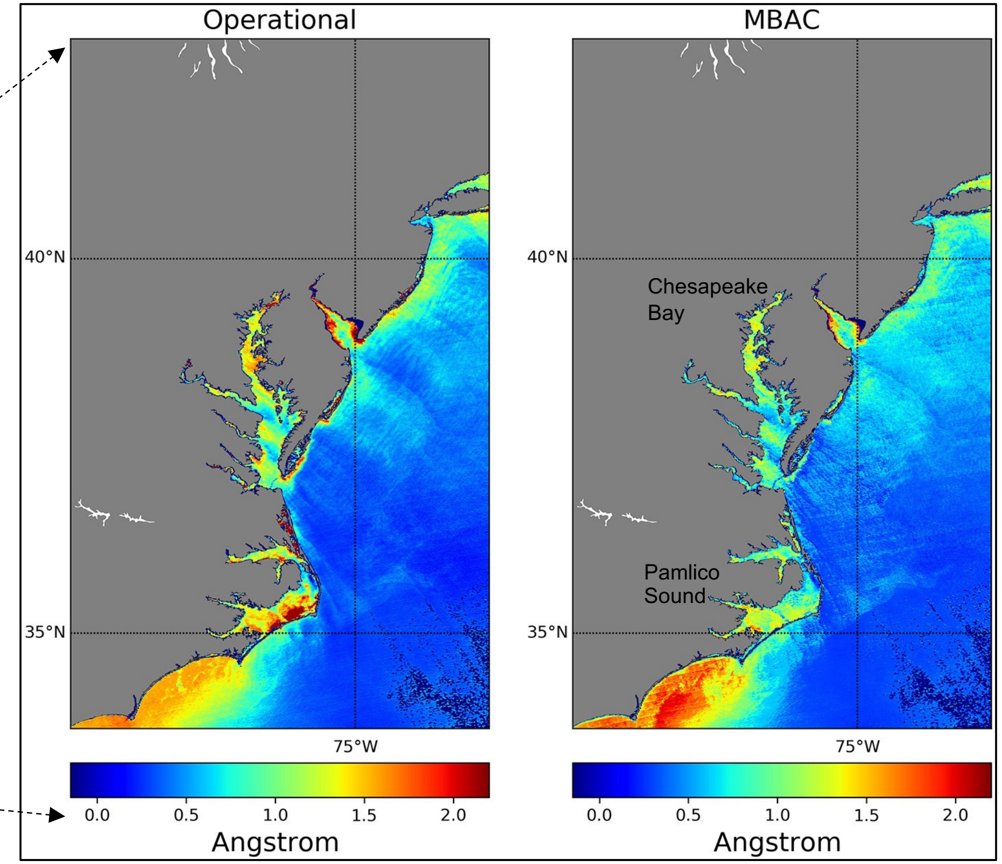




Knaeps et al. 2015 RSE

Application to MODIS- Aqua

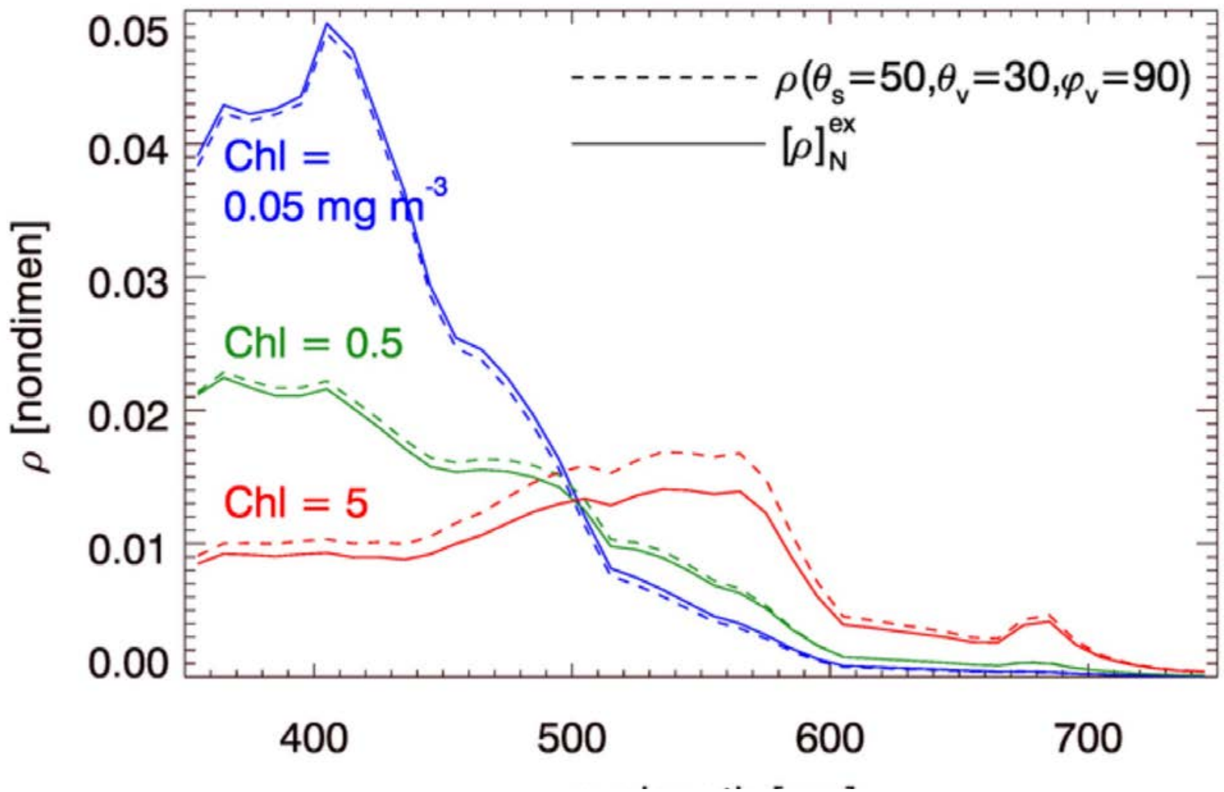




- ✓ MBAC retrievals are similar to the operational algorithm, except in turbid coastal regions.
- ✓ That is due to the difference in the retrieved aerosols models.
- ✓ Turbid waters over-estimate the aerosol reflectance (i.e., angstrom).

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.

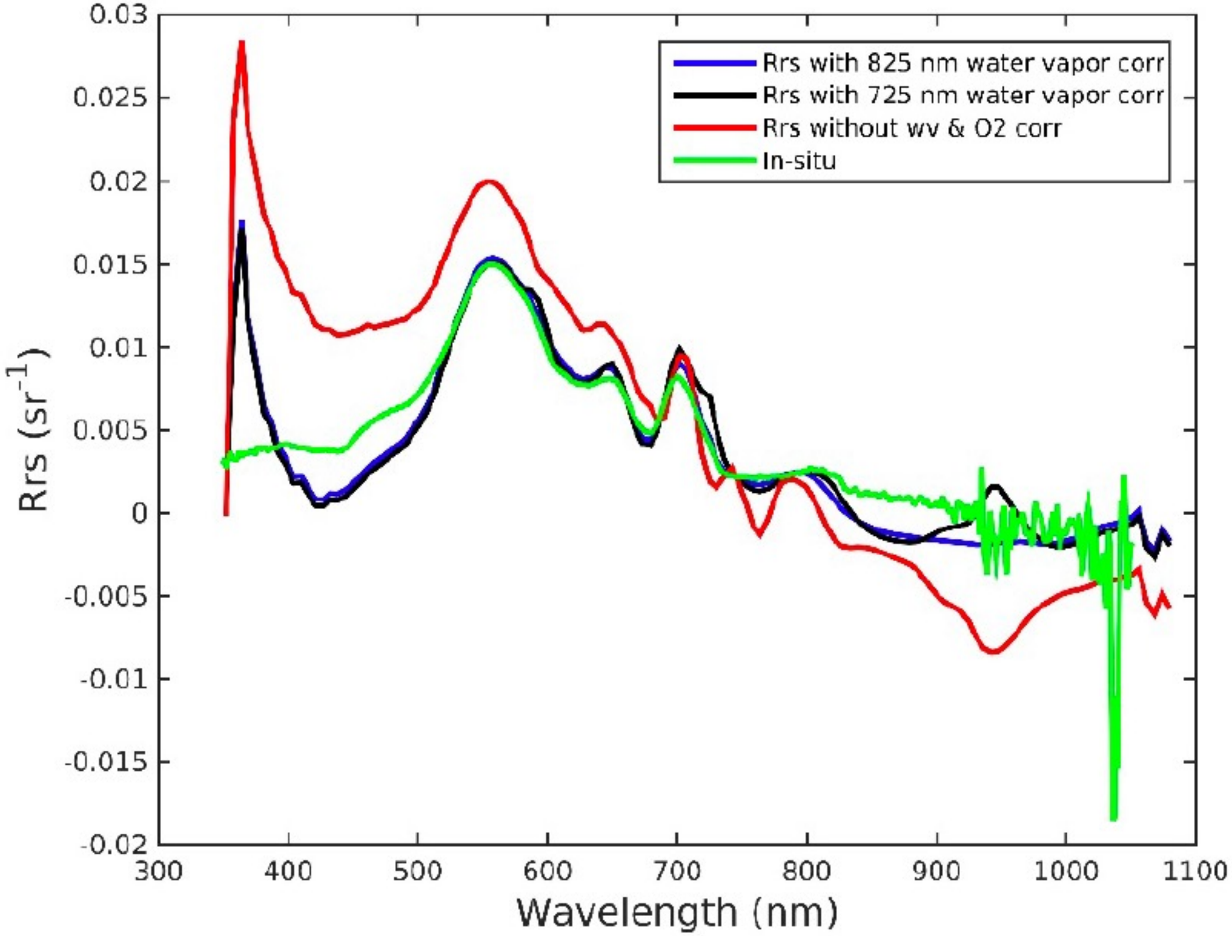


$$[\rho_w]_N^{ex} \equiv \frac{\pi}{F_o}[L_w]_N^{ex}$$

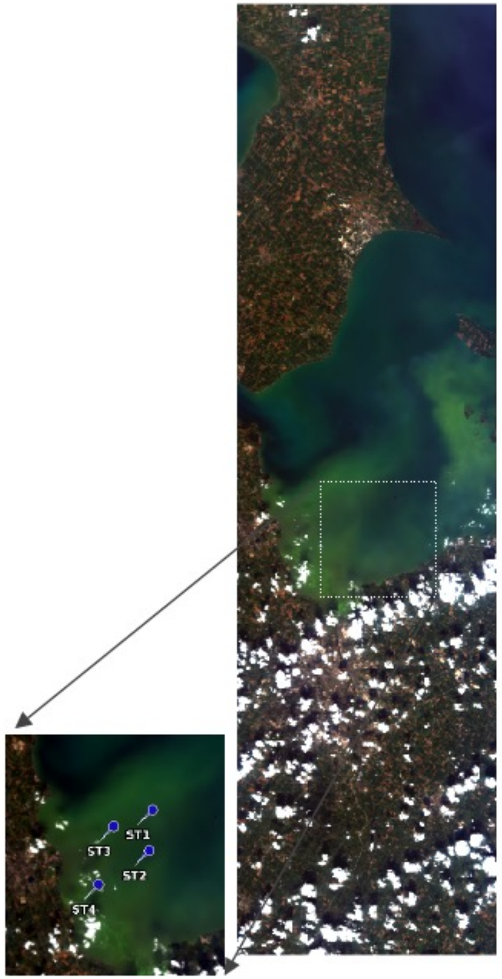
$$= \left\{ \frac{\pi}{F_o \cos\theta_s\, t(\theta_s)} \frac{\mathfrak{R}_o(W)}{\mathfrak{R}(\theta'_v, W)} \frac{f_o(\mathrm{ATM}, W, \mathrm{IOP})}{Q_o(\mathrm{ATM}, W, \mathrm{IOP})} \left[\frac{f(\theta_s, \mathrm{ATM}, W, \mathrm{IOP})}{Q(\theta_s, \theta'_v, \phi, \mathrm{ATM}, W, \mathrm{IOP})} \right]^{-1} \right\} \times$$

$$L_w(\theta_s, \theta_v, \phi)\,.$$

Demonstration of Hyperspectral Rrs(λ) Retrieval from HICO, including correction for atmospheric water vapor

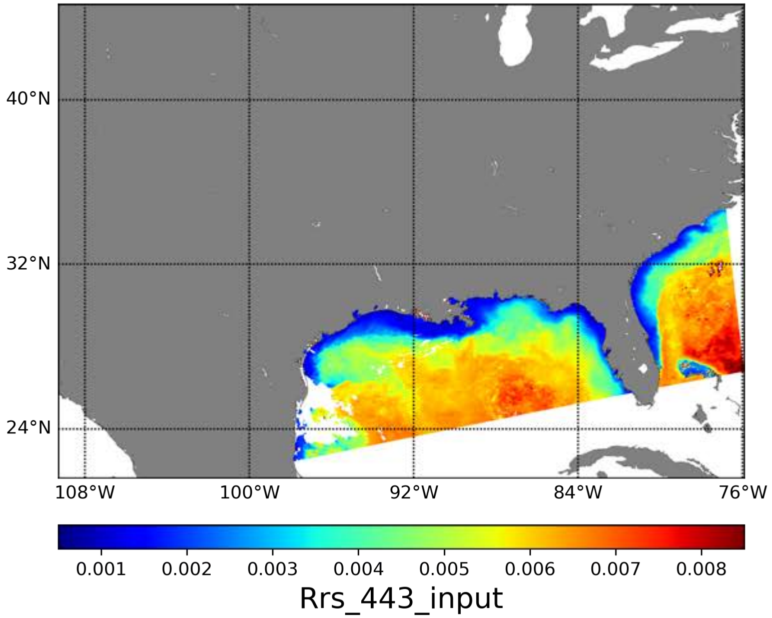


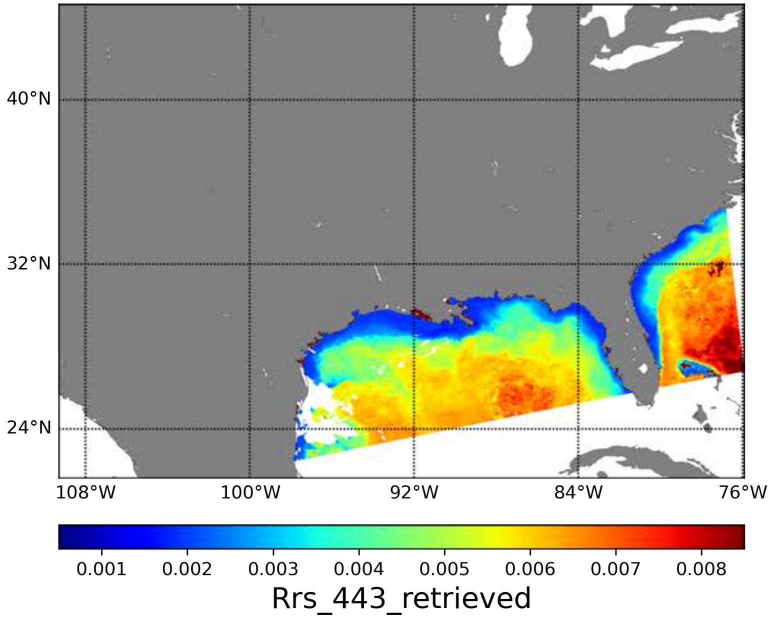
True color

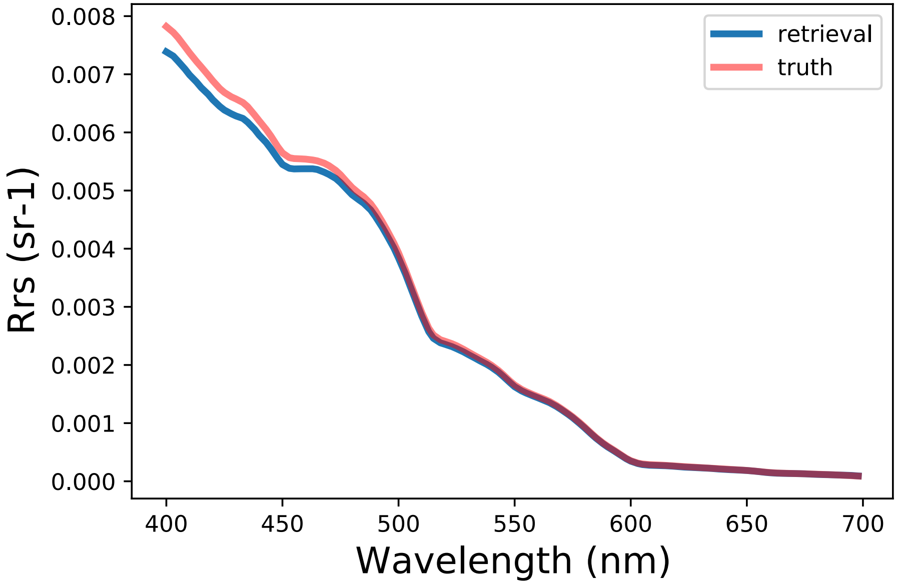


Example over Lake Erie. In-situ measurements provided by Tim Moore (UNH), obtained from SeaBASS

Putting it all together
Testing HS AC on simulated OCI data

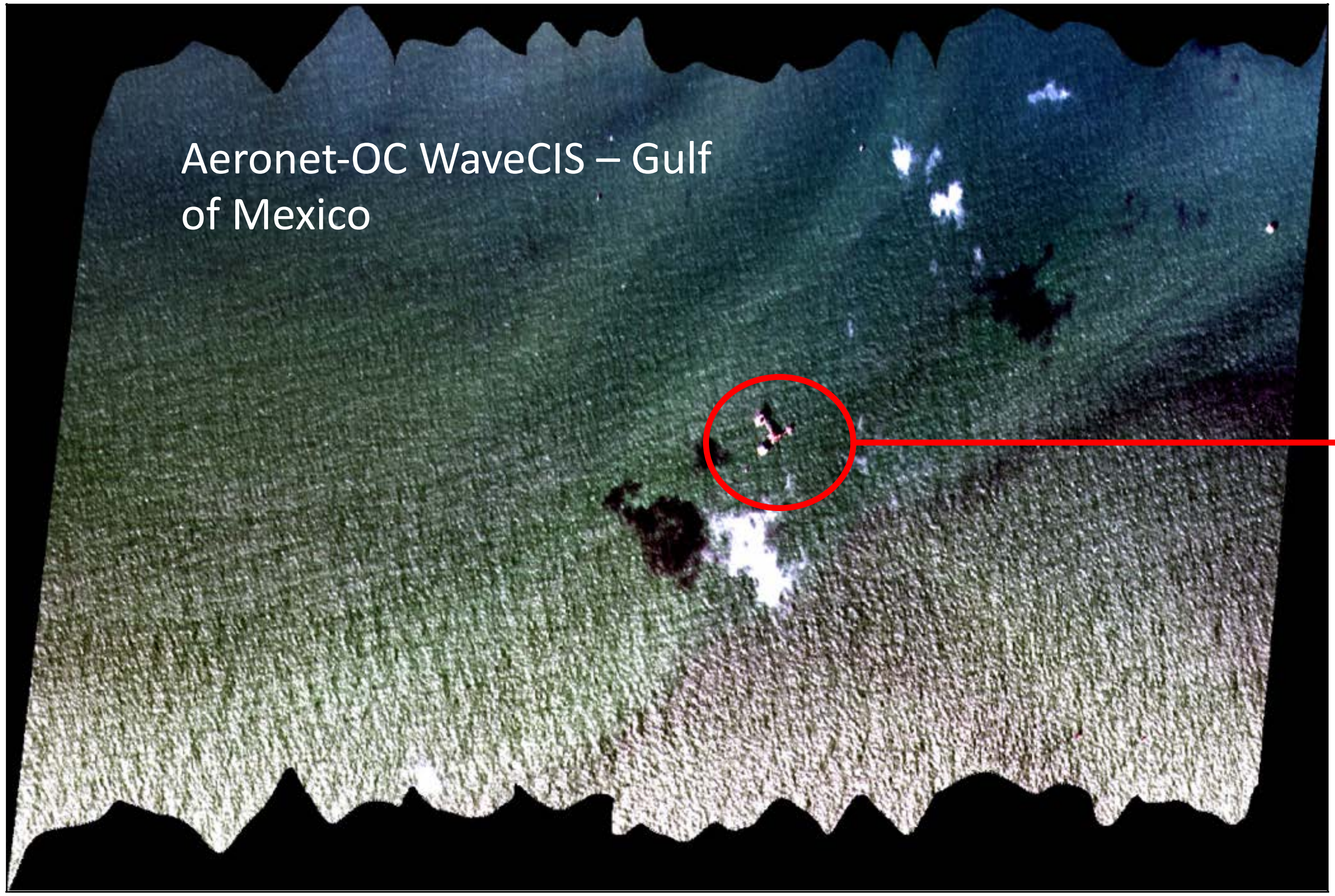


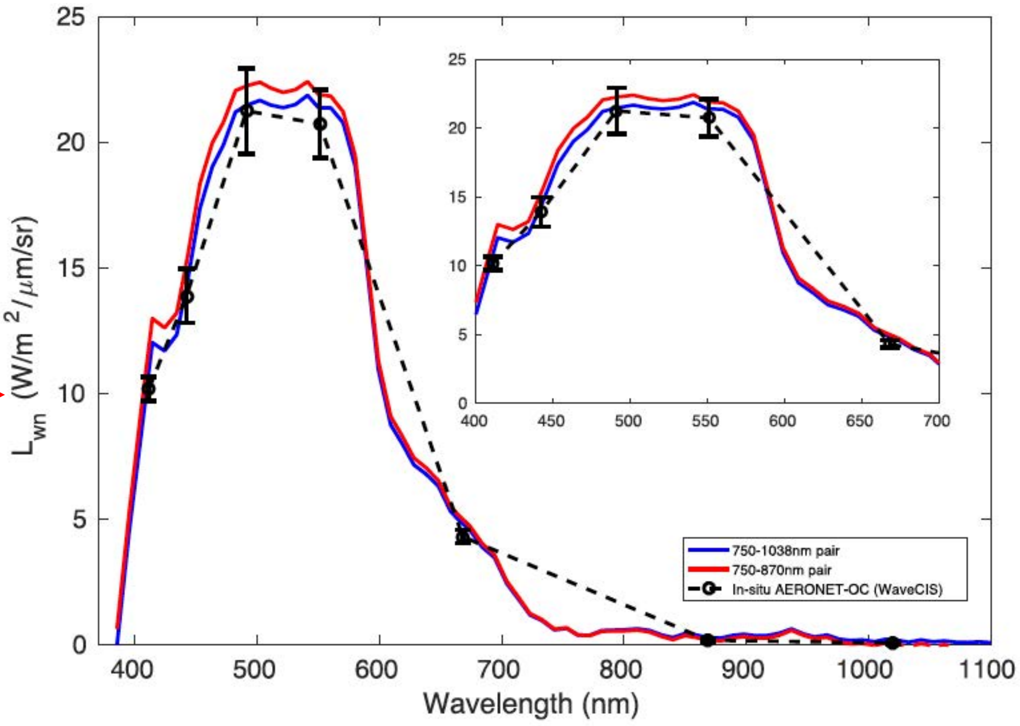




Example retrieval of Rrs
from PyTOAST simulations

HS AC from airborne data - AVIRIS





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.

Ryan Vandermeulen